

```

chain nodes :
  13
ring nodes :
  1 2 3 4 5 6 7 8 9 10 11 12 17 18 19 20 21 22
ring/chain nodes :
  15
chain bonds :
  3-9 7-13 8-18
ring bonds :
  1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 17-18 17-22 18-19 19-20
  20-21 21-22
exact/norm bonds :
  7-8 7-12 7-13 8-9 8-18 9-10 10-11 11-12
exact bonds :
  3-9
normalized bonds :
  1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-22 18-19 19-20 20-21 21-22
isolated ring systems :
  containing 1 : 7 :

```

```

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom

```

10/582,826

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 1839

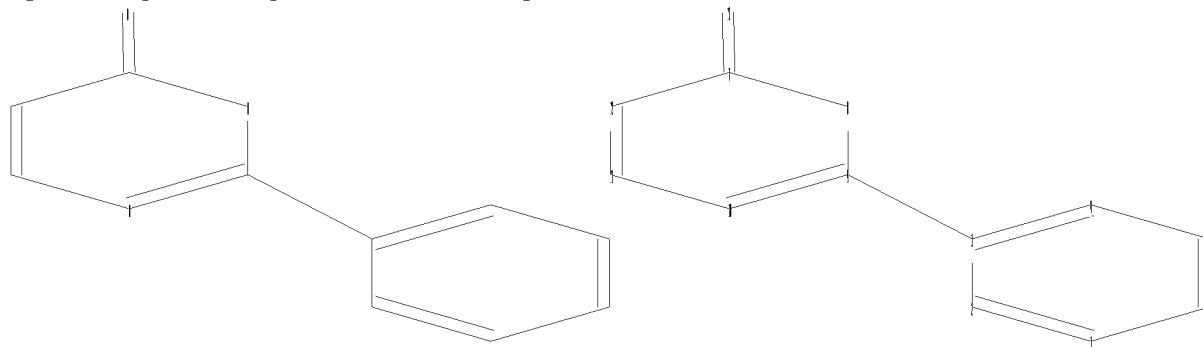
L1 SCREEN CREATED

=> screen 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

L2 SCREEN CREATED

=>

Uploading C:\Program Files\Stnexp\Queries\10582826.str



chain nodes :

13

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds :

3-9 7-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

7-8 7-12 7-13 8-9 9-10 10-11 11-12

exact bonds :

3-9

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 7 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS

L3 STRUCTURE UPLOADED

=> que L3 AND L1 NOT L2

L4 QUE L3 AND L1 NOT L2

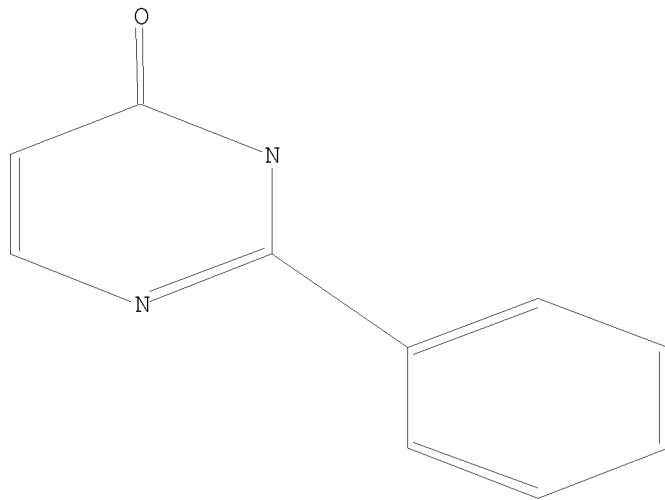
=> d 14

L4 HAS NO ANSWERS

L1 SCR 1839

L2 SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

L3 STR



Structure attributes must be viewed using STN Express query preparation.

L4 QUE L3 AND L1 NOT L2

=> s 14 sss sam

SAMPLE SEARCH INITIATED 14:00:11 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 4763 TO ITERATE

42.0% PROCESSED 2000 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 91121 TO 99399

PROJECTED ANSWERS: 6846 TO 9252

L5 50 SEA SSS SAM L3 AND L1 NOT L2

=> =>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 1839

10/582,826

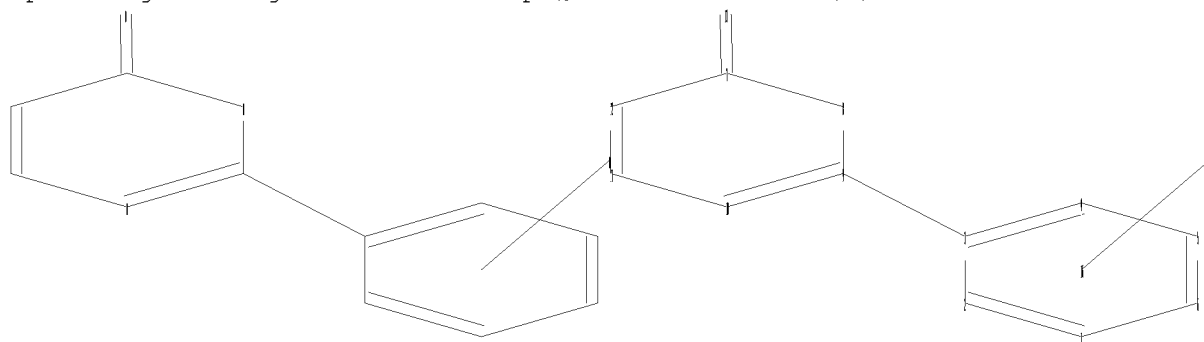
L6 SCREEN CREATED

=> screen 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

L7 SCREEN CREATED

=>

Uploading C:\Program Files\Stnexp\Queries\10582826 (a).str



chain nodes :

13

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

ring/chain nodes :

15

chain bonds :

3-9 7-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

7-8 7-12 7-13 8-9 9-10 10-11 11-12

exact bonds :

3-9

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 : 7 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 15:CLASS 16:Atom

L8 STRUCTURE UPLOADED

=> que L8 AND L6 NOT L7

10/582,826

L9 QUE L8 AND L6 NOT L7

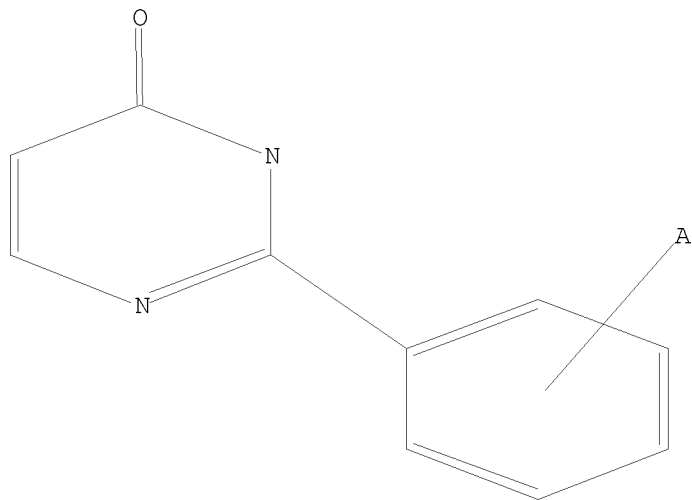
=> d 19

L9 HAS NO ANSWERS

L6 SCR 1839

L7 SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

L8 STR



Structure attributes must be viewed using STN Express query preparation.

L9 QUE L8 AND L6 NOT L7

=> s 19 sss sam

SAMPLE SEARCH INITIATED 14:03:12 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 4763 TO ITERATE

42.0% PROCESSED 2000 ITERATIONS

50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 91121 TO 99399

PROJECTED ANSWERS: 4009 TO 5897

L10 50 SEA SSS SAM L8 AND L6 NOT L7

=>Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 1839

L11 SCREEN CREATED

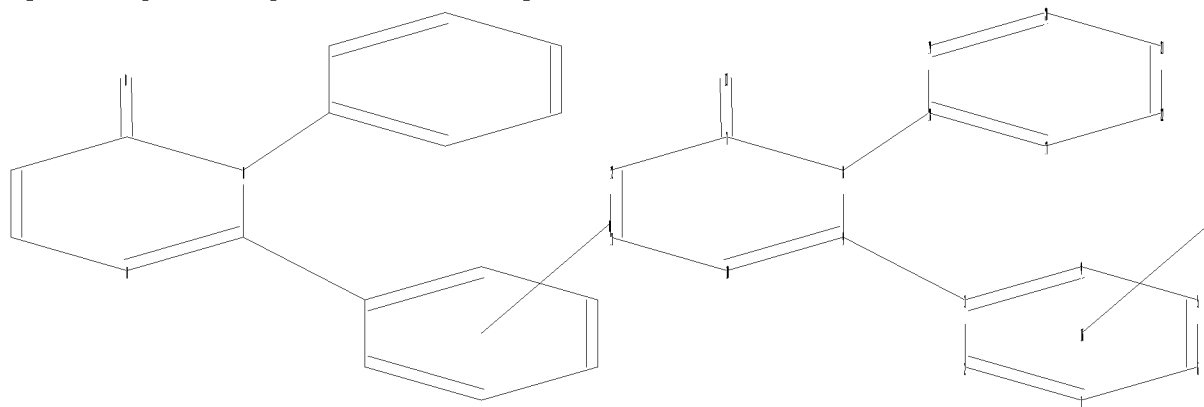
10/582,826

=> screen 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

L12 SCREEN CREATED

=>

Uploading C:\Program Files\Stnexp\Queries\10582826 (claim 2).str



chain nodes :

13

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 17 18 19 20 21 22

ring/chain nodes :

15

chain bonds :

3-9 7-13 8-18

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 17-18 17-22
18-19 19-20 20-21 21-22

exact/norm bonds :

7-8 7-12 7-13 8-9 8-18 9-10 10-11 11-12

exact bonds :

3-9

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-22 18-19 19-20 20-21 21-22

isolated ring systems :

containing 1 : 7 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom
21:Atom 22:Atom

L13 STRUCTURE UPLOADED

10/582,826

=> que L13 AND L11 NOT L12

L14 QUE L13 AND L11 NOT L12

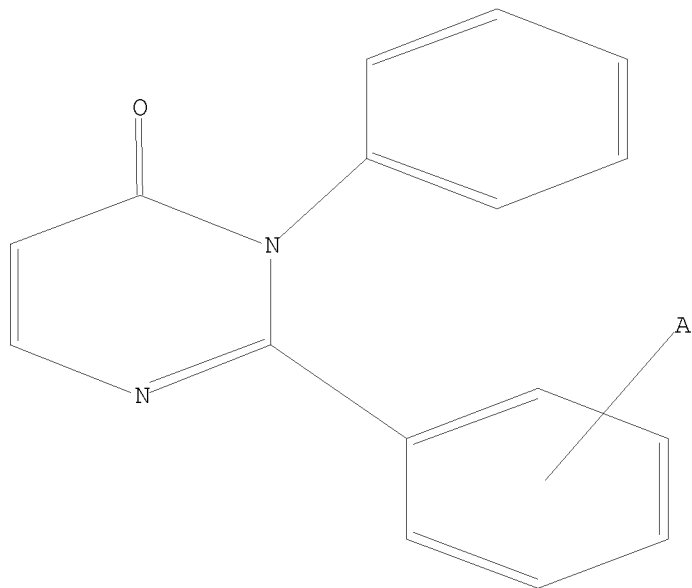
=> d l14

L14 HAS NO ANSWERS

L11 SCR 1839

L12 SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

L13 STR



Structure attributes must be viewed using STN Express query preparation.

L14 QUE L13 AND L11 NOT L12

=> s l14 sss sam

SAMPLE SEARCH INITIATED 14:06:18 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 704 TO ITERATE

100.0% PROCESSED 704 ITERATIONS

12 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 12489 TO 15671

PROJECTED ANSWERS: 33 TO 447

L15 12 SEA SSS SAM L13 AND L11 NOT L12

=> => s l14 sss ful

FULL SEARCH INITIATED 14:07:05 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 13552 TO ITERATE

100.0% PROCESSED 13552 ITERATIONS

221 ANSWERS

10/582,826

SEARCH TIME: 00.00.01

L16 221 SEA SSS FUL L13 AND L11 NOT L12

=> => s l16

L17 17 L16

=> d l17 1-17 bib,ab,hitstr

L17 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

AN 2007:1454797 CAPLUS

DN 148:79051

TI Preparation of diaryl pyrimidinones and related compounds as CB1 modulators

IN Li, Hongbin; Yuan, Jun; Wustrow, David J.

PA Neurogen Corporation, USA

SO PCT Int. Appl., 89pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2007146761	A2	20071221	WO 2007-US70676	20070608
	WO 2007146761	A3	20081030		
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	RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA			

PRAI US 2006-804451P P 20060612

OS MARPAT 148:79051

AB The title compds. I [A = CR1 or N; Ar1, Ar2 = (un)substituted Ph, naphthyl and 5-10 membered heteroaryl; R1 = H, OH, NO2, alkyl, etc.; R2 = alkenyl, cycloalkylalkyl, alkoxy, etc.] that may be used to modulate CB1 activity in vivo or in vitro, and are particularly useful in the treatment of conditions responsive to CB1 modulation in humans, domesticated companion animals and livestock animals, including appetite disorders, obesity and dependency disorders (no data), were prepared and disclosed. E.g., a multi-step synthesis of II, starting from 4-trifluoromethylaniline and 2-chlorobenzoyl chloride was described. Pharmaceutical compns. comprising the compound I alone or in combination with other therapeutic agent, and methods for using them to treat CB1 receptor-mediated disorders are provided, as are methods for using such ligands for receptor localization studies and various in vitro assays.

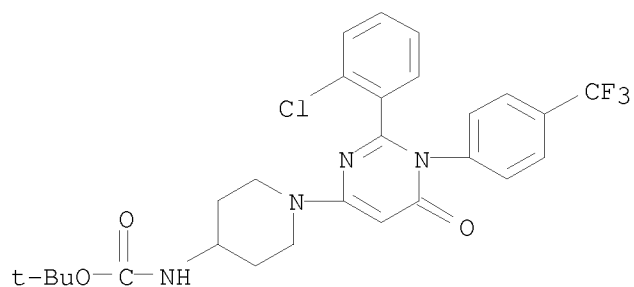
IT 960320-37-0P

RL: PAC (Pharmacological activity); PRPH (Prophetic); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of diaryl pyrimidinone compds. as CB1 receptor modulators for treating CB1 receptor-mediated diseases)

RN 960320-37-0 CAPLUS

CN Carbamic acid, N-[1-[2-(2-chlorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



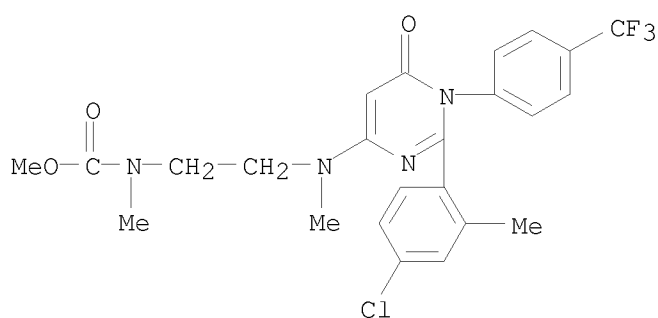
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 960321-60-2P 960321-61-3P 960321-62-4P
 960321-63-5P 960321-64-6P

RL: PAC (Pharmacological activity); PRPH (Prophetic); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of diaryl pyrimidinone compds. as CB1 receptor modulators for treating CB1 receptor-mediated diseases)

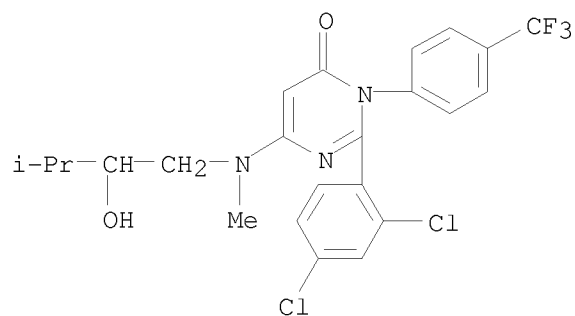
RN 960321-57-7 CAPLUS

CN Carbamic acid, N-[2-[[2-(4-chloro-2-methylphenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]methylamino]ethyl]-N-methyl-, methyl ester (CA INDEX NAME)



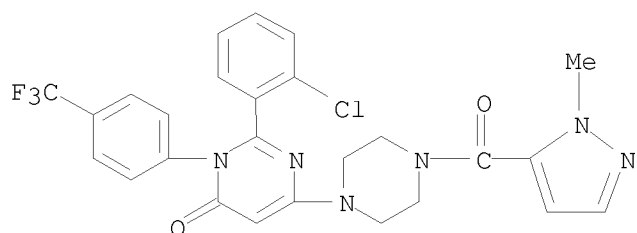
RN 960321-58-8 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2,4-dichlorophenyl)-6-[(2-hydroxy-3-methylbutyl)methylamino]-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



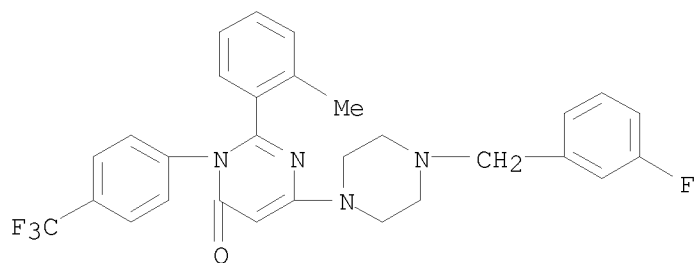
RN 960321-59-9 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2-chlorophenyl)-6-[4-[(1-methyl-1H-pyrazol-5-yl)carbonyl]-1-piperazinyl]-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



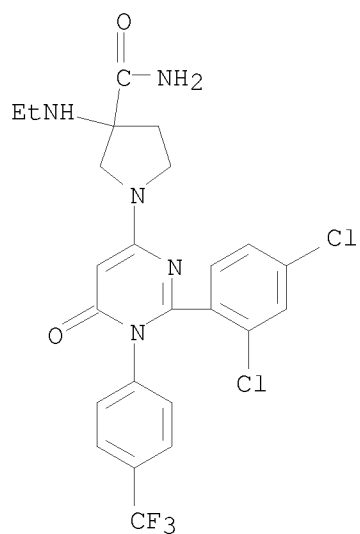
RN 960321-60-2 CAPLUS

CN 4(3H)-Pyrimidinone, 6-[4-[(3-fluorophenyl)methyl]-1-piperazinyl]-2-(2-methylphenyl)-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



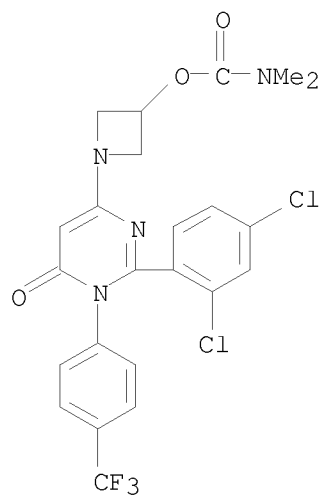
RN 960321-61-3 CAPLUS

CN 3-Pyrrolidinecarboxamide, 1-[2-(2,4-dichlorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-3-(ethylamino)- (CA INDEX NAME)



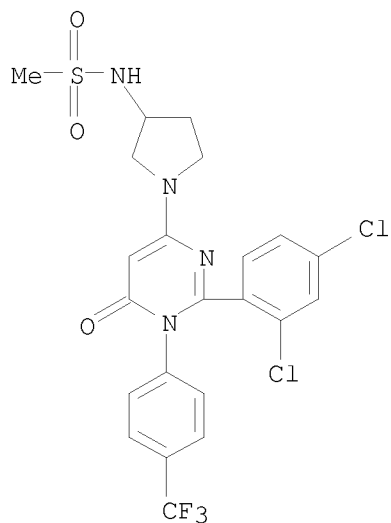
RN 960321-62-4 CAPLUS

CN Carbamic acid, N,N-dimethyl-, 1-[2-(2,4-dichlorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-3-azetidiny ester (CA INDEX NAME)



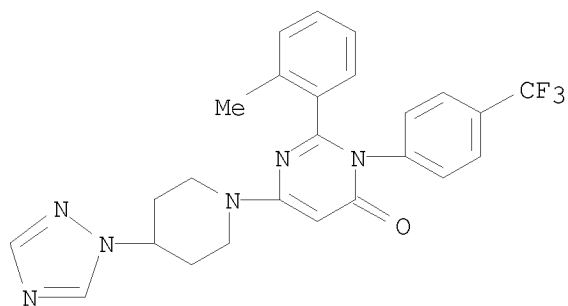
RN 960321-63-5 CAPLUS

CN Methanesulfonamide, N-[1-[2-(2,4-dichlorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-3-pyrrolidinyl]- (CA INDEX NAME)



RN 960321-64-6 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2-methylphenyl)-6-[4-(1H-1,2,4-triazol-1-yl)-1-piperidinyl]-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)

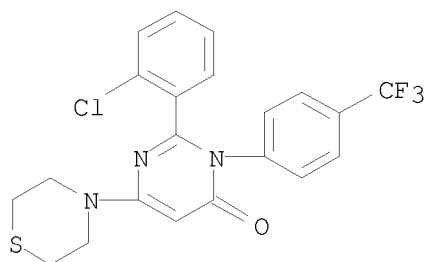


IT 960320-41-6P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of diaryl pyrimidinone compds. as CB1 receptor modulators for treating CB1 receptor-mediated diseases)

RN 960320-41-6 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2-chlorophenyl)-6-(4-thiomorpholinyl)-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



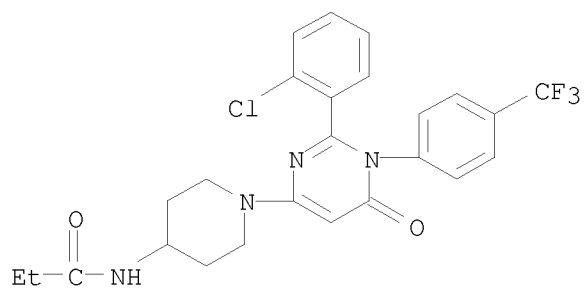
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 960321-52-2P 960321-53-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(preparation of diaryl pyrimidinone compds. as CB1 receptor modulators for
 treating CB1 receptor-mediated diseases)

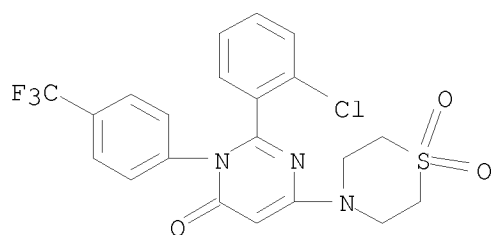
RN 960320-39-2 CAPLUS

CN Propanamide, N-[1-[2-(2-chlorophenyl)-1,6-dihydro-6-oxo-1-[4-
 (trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]- (CA INDEX NAME)



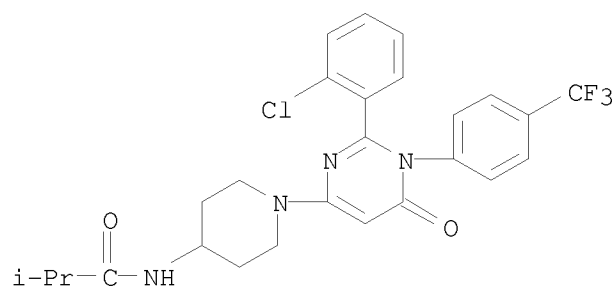
RN 960320-42-7 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2-chlorophenyl)-6-(1,1-dioxido-4-thiomorpholinyl)-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



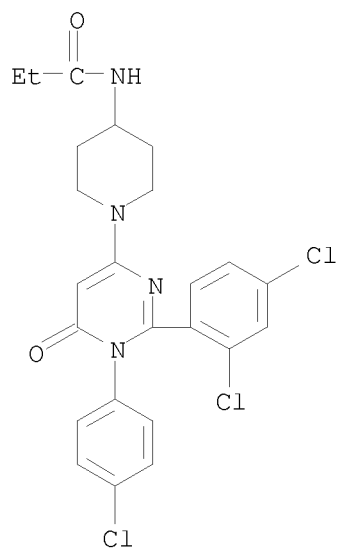
RN 960320-44-9 CAPLUS

CN Propanamide, N-[1-[2-(2-chlorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-2-methyl- (CA INDEX NAME)



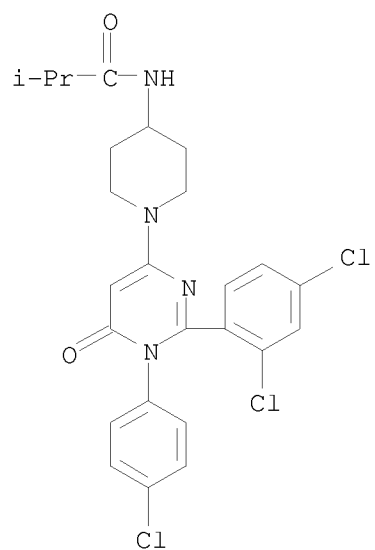
RN 960320-45-0 CAPLUS

CN Propanamide, N-[1-[1-(4-chlorophenyl)-2-(2,4-dichlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-4-piperidinyl]- (CA INDEX NAME)



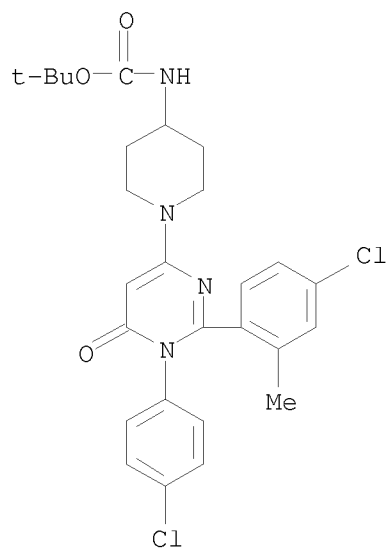
RN 960320-46-1 CAPLUS

CN Propanamide, N-[1-[1-(4-chlorophenyl)-2-(2,4-dichlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-4-piperidiny]-2-methyl- (CA INDEX NAME)



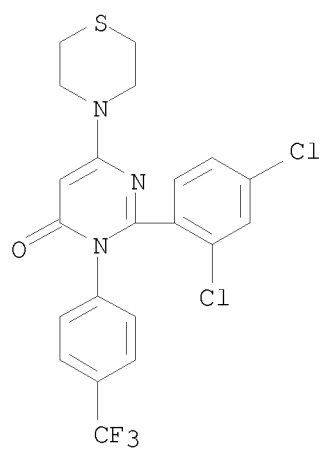
RN 960320-49-4 CAPLUS

CN Carbamic acid, N-[1-[2-(4-chloro-2-methylphenyl)-1-(4-chlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-4-piperidiny]-, 1,1-dimethylethyl ester (CA INDEX NAME)



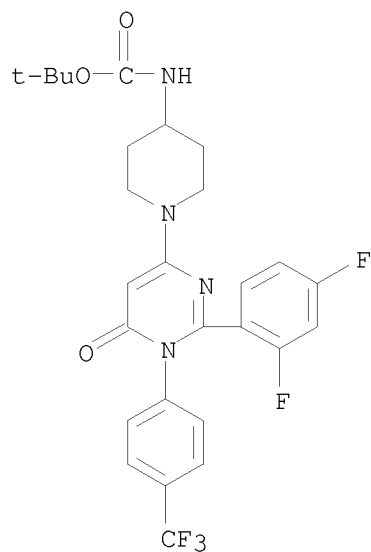
RN 960320-50-7 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2,4-dichlorophenyl)-6-(4-thiomorpholinyl)-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



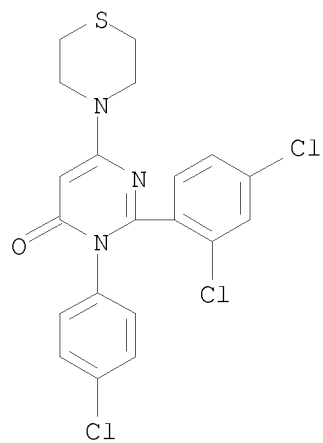
RN 960320-51-8 CAPLUS

CN Carbamic acid, N-[1-[2-(2,4-difluorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



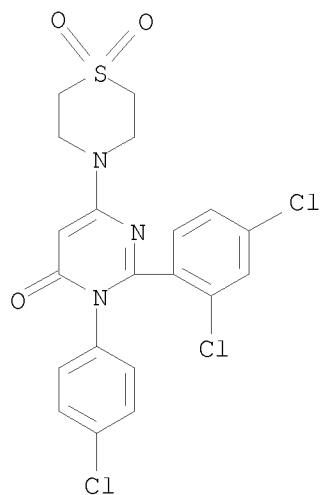
RN 960320-52-9 CAPLUS

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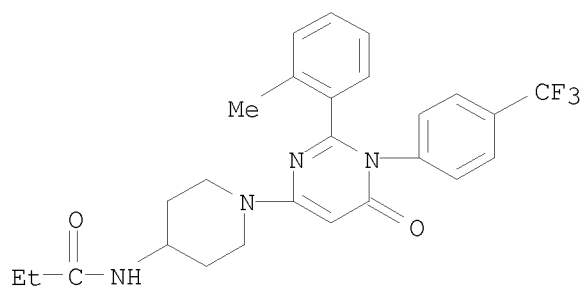


RN 960320-54-1 CAPLUS

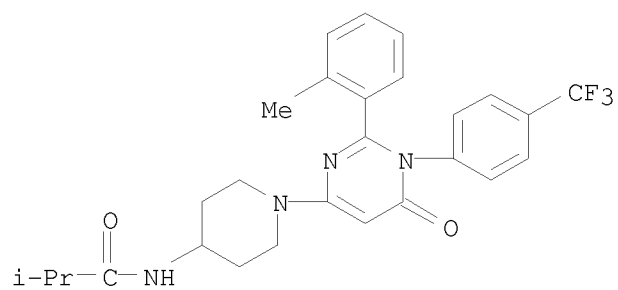
CN 4(3H)-Pyrimidinone, 3-(4-chlorophenyl)-2-(2,4-dichlorophenyl)-6-(1,1-dioxido-4-thiomorpholinyl)- (CA INDEX NAME)



RN 960320-56-3 CAPLUS
 CN Propanamide, N-[1-[1,6-dihydro-2-(2-methylphenyl)-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]- (CA INDEX NAME)

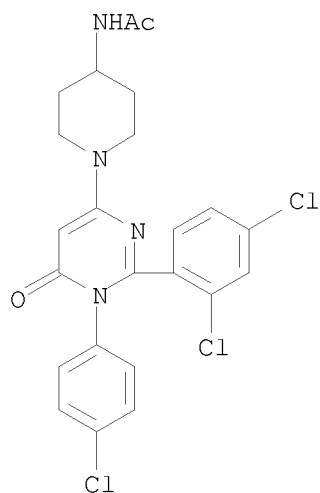


RN 960320-57-4 CAPLUS
 CN Propanamide, N-[1-[1,6-dihydro-2-(2-methylphenyl)-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-2-methyl- (CA INDEX NAME)



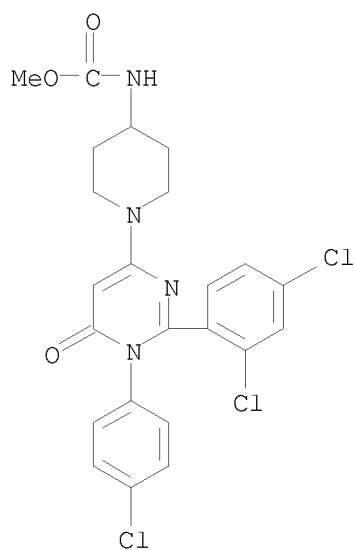
RN 960320-60-9 CAPLUS
 CN Acetamide, N-[1-[1-(4-chlorophenyl)-2-(2,4-dichlorophenyl)-1,6-dihydro-6-

oxo-4-pyrimidinyl]-4-piperidinyl]- (CA INDEX NAME)



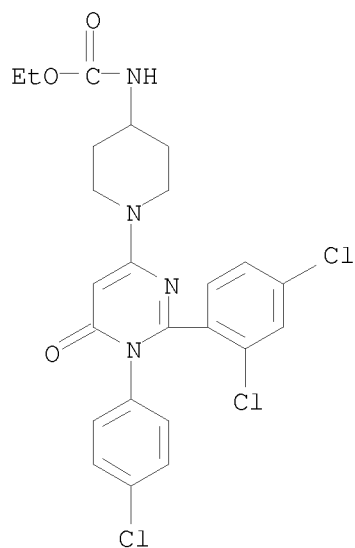
RN 960320-61-0 CAPLUS

CN Carbamic acid, N-[1-[1-(4-chlorophenyl)-2-(2,4-dichlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-4-piperidinyl]-, methyl ester (CA INDEX NAME)



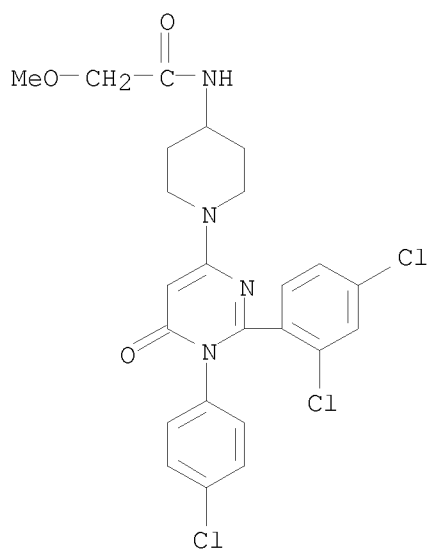
RN 960320-62-1 CAPLUS

CN Carbamic acid, N-[1-[1-(4-chlorophenyl)-2-(2,4-dichlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-4-piperidinyl]-, ethyl ester (CA INDEX NAME)



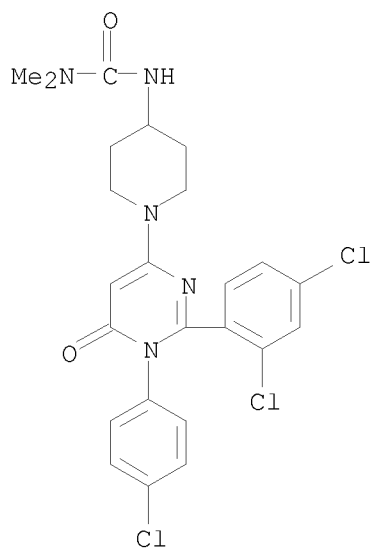
RN 960320-63-2 CAPLUS

CN Acetamide, N-[1-[1-(4-chlorophenyl)-2-(2,4-dichlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-4-piperidinyl]-2-methoxy- (CA INDEX NAME)

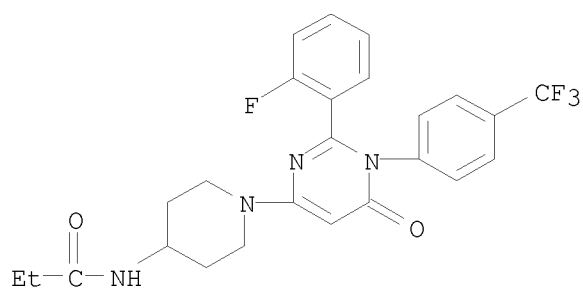


RN 960320-64-3 CAPLUS

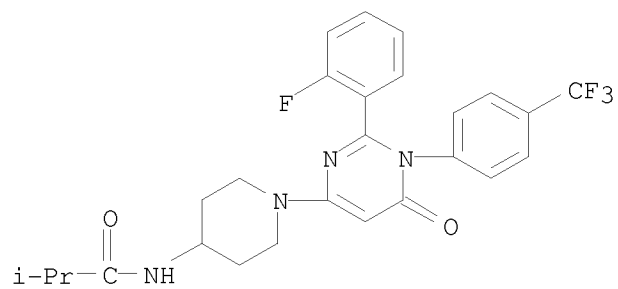
CN Urea, N'-[1-[1-(4-chlorophenyl)-2-(2,4-dichlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-4-piperidinyl]-N,N-dimethyl- (CA INDEX NAME)



RN 960320-65-4 CAPLUS
 CN Propanamide, N-[1-[2-(2-fluorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]- (CA INDEX NAME)

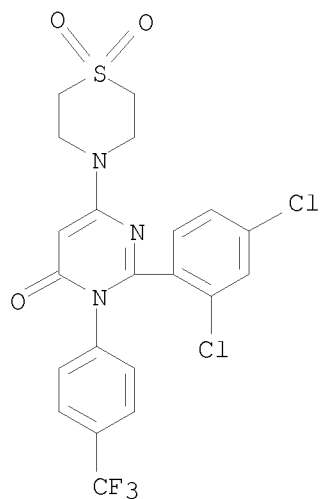


RN 960320-66-5 CAPLUS
 CN Propanamide, N-[1-[2-(2-fluorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-2-methyl- (CA INDEX NAME)



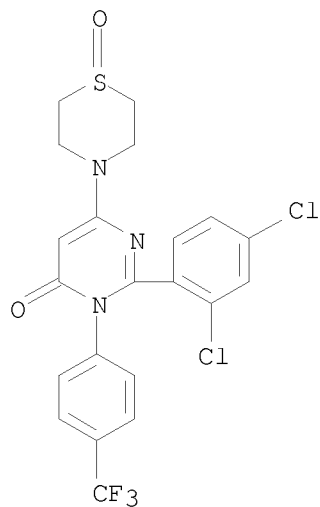
RN 960320-69-8 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2,4-dichlorophenyl)-6-(1,1-dioxido-4-thiomorpholinyl)-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



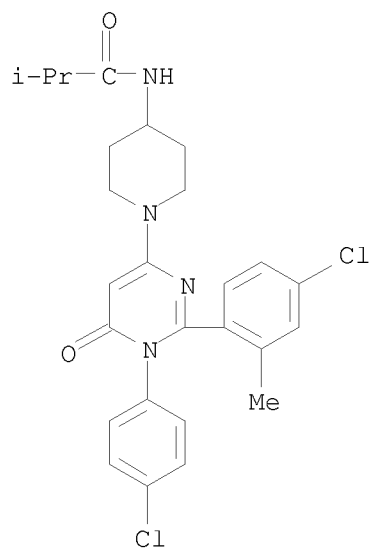
RN 960320-70-1 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2,4-dichlorophenyl)-6-(1-oxido-4-thiomorpholinyl)-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



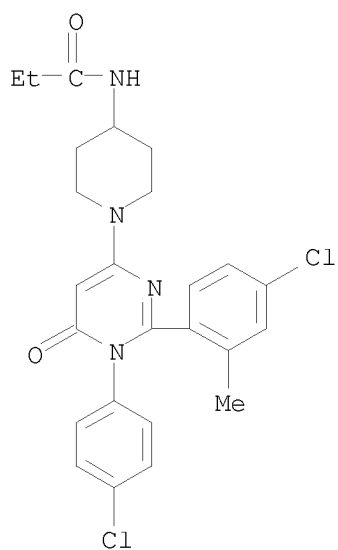
RN 960320-71-2 CAPLUS

CN Propanamide, N-[1-[2-(4-chloro-2-methylphenyl)-1-(4-chlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-4-piperidinyl]-2-methyl- (CA INDEX NAME)



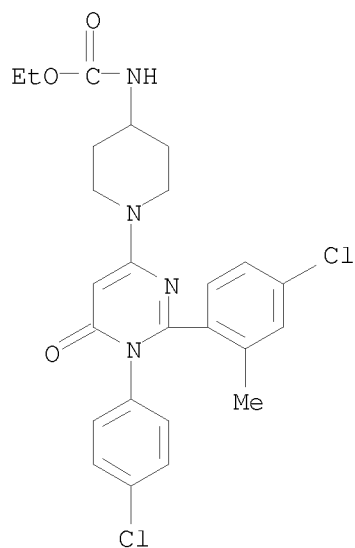
RN 960320-72-3 CAPLUS

CN Propanamide, N-[1-[2-(4-chloro-2-methylphenyl)-1-(4-chlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-4-piperidinyl]- (CA INDEX NAME)



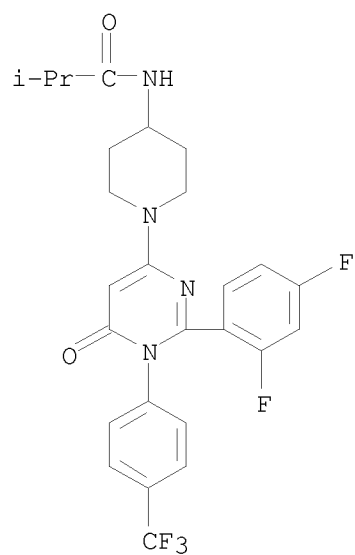
RN 960320-73-4 CAPLUS

CN Carbamic acid, N-[1-[2-(4-chloro-2-methylphenyl)-1-(4-chlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-4-piperidinyl]-, ethyl ester (CA INDEX NAME)



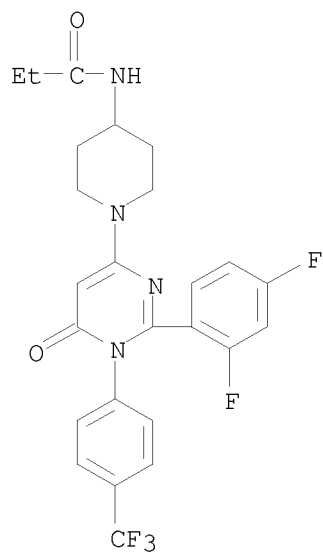
RN 960320-74-5 CAPLUS

CN Propanamide, N-[1-[2-(2,4-difluorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-2-methyl- (CA INDEX NAME)



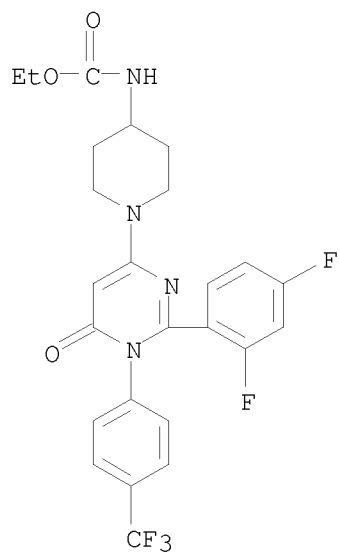
RN 960320-75-6 CAPLUS

CN Propanamide, N-[1-[2-(2,4-difluorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]- (CA INDEX NAME)



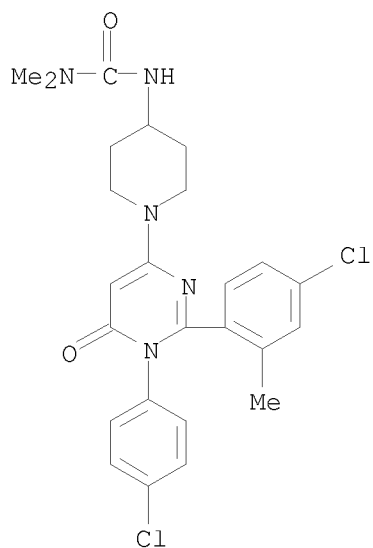
RN 960320-76-7 CAPLUS

CN Carbamic acid, N-[1-[2-(2,4-difluorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-, ethyl ester (CA INDEX NAME)



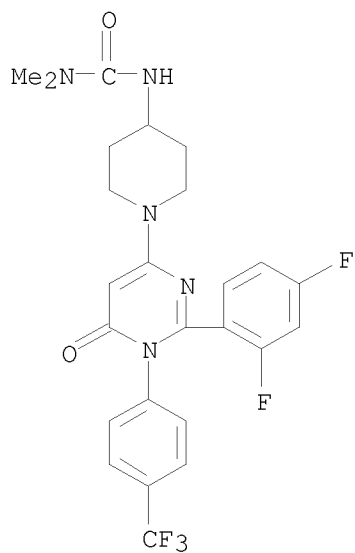
RN 960320-77-8 CAPLUS

CN Urea, N'-[1-[2-(4-chloro-2-methylphenyl)-1-(4-chlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-4-piperidinyl]-N,N-dimethyl- (CA INDEX NAME)



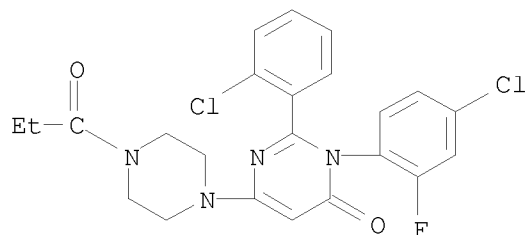
RN 960320-78-9 CAPLUS

CN Urea, N'-[1-[2-(2,4-difluorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-N,N-dimethyl- (CA INDEX NAME)



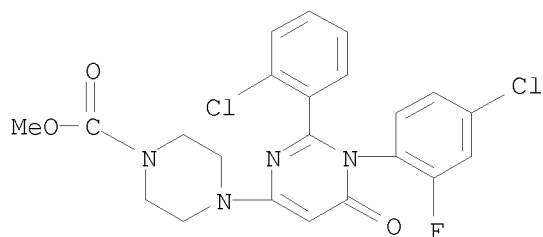
RN 960320-79-0 CAPLUS

CN 4(3H)-Pyrimidinone, 3-(4-chloro-2-fluorophenyl)-2-(2-chlorophenyl)-6-[4-(1-oxopropyl)-1-piperazinyl]- (CA INDEX NAME)



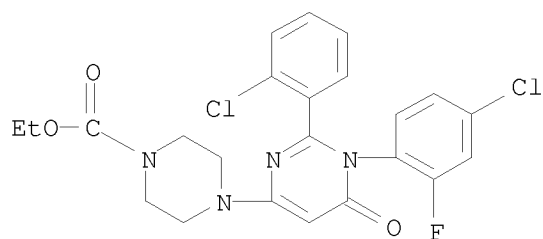
RN 960320-80-3 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[1-(4-chloro-2-fluorophenyl)-2-(2-chlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-, methyl ester (CA INDEX NAME)



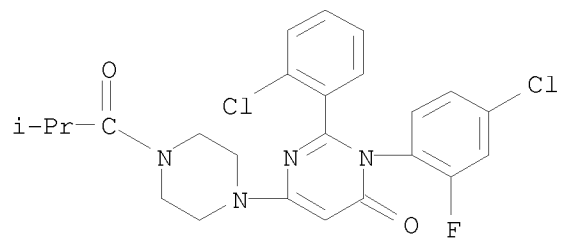
RN 960320-81-4 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[1-(4-chloro-2-fluorophenyl)-2-(2-chlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-, ethyl ester (CA INDEX NAME)



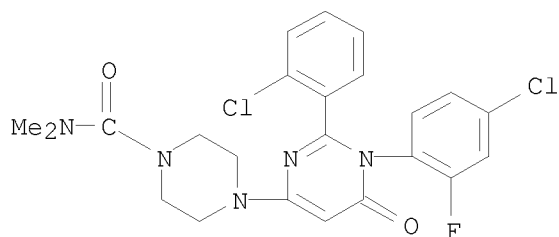
RN 960320-82-5 CAPLUS

CN 4(3H)-Pyrimidinone, 3-(4-chloro-2-fluorophenyl)-2-(2-chlorophenyl)-6-[4-(2-methyl-1-oxopropyl)-1-piperazinyl]- (CA INDEX NAME)



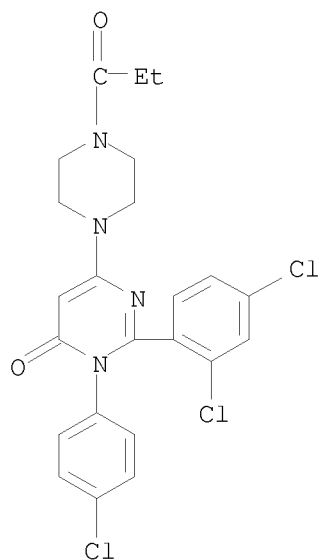
RN 960320-83-6 CAPLUS

CN 1-Piperazinecarboxamide, 4-[1-(4-chloro-2-fluorophenyl)-2-(2-chlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-N,N-dimethyl- (CA INDEX NAME)



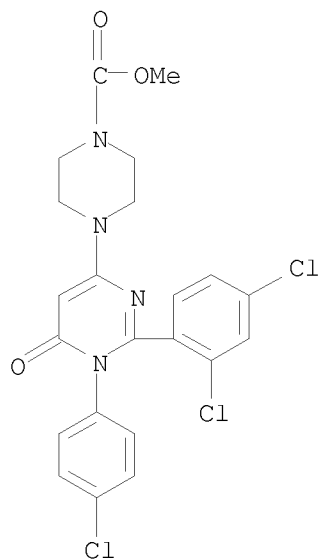
RN 960320-84-7 CAPLUS

CN 4(3H)-Pyrimidinone, 3-(4-chlorophenyl)-2-(2,4-dichlorophenyl)-6-[4-(1-oxopropyl)-1-piperazinyl]- (CA INDEX NAME)



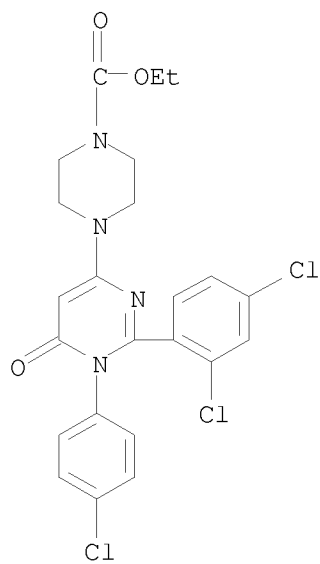
RN 960320-85-8 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[1-(4-chlorophenyl)-2-(2,4-dichlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-, methyl ester (CA INDEX NAME)



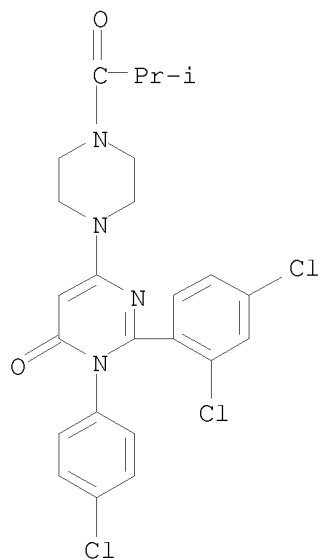
RN 960320-86-9 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[1-(4-chlorophenyl)-2-(2,4-dichlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-, ethyl ester (CA INDEX NAME)



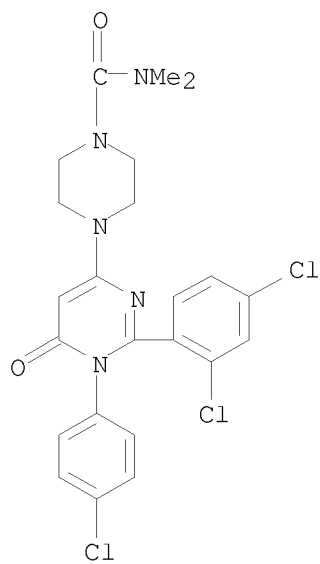
RN 960320-87-0 CAPLUS

CN 4(3H)-Pyrimidinone, 3-(4-chlorophenyl)-2-(2,4-dichlorophenyl)-6-[4-(2-methyl-1-oxopropyl)-1-piperazinyl]- (CA INDEX NAME)



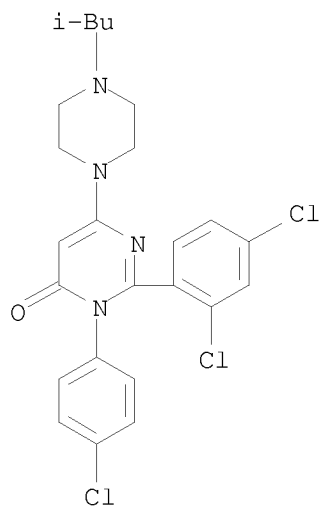
RN 960320-88-1 CAPLUS

CN 1-Piperazinecarboxamide, 4-[1-(4-chlorophenyl)-2-(2,4-dichlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-N,N-dimethyl- (CA INDEX NAME)



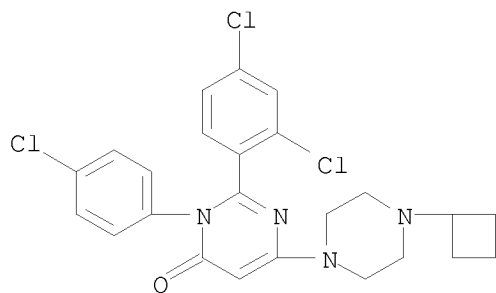
RN 960320-89-2 CAPLUS

CN 4(3H)-Pyrimidinone, 3-(4-chlorophenyl)-2-(2,4-dichlorophenyl)-6-[4-(2-methylpropyl)-1-piperazinyl]- (CA INDEX NAME)



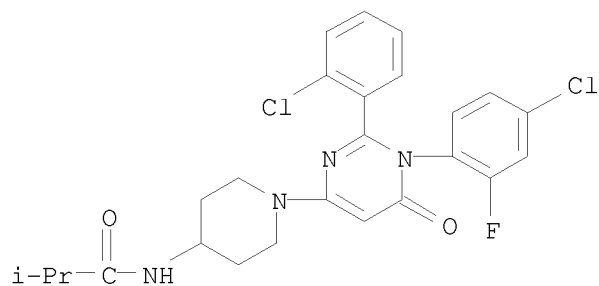
RN 960320-90-5 CAPLUS

CN 4(3H)-Pyrimidinone, 3-(4-chlorophenyl)-6-(4-cyclobutyl-1-piperazinyl)-2-(2,4-dichlorophenyl)- (CA INDEX NAME)



RN 960320-91-6 CAPLUS

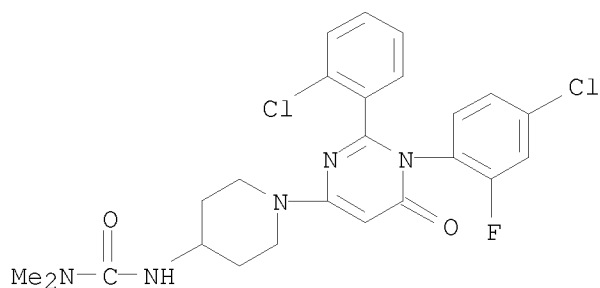
CN Propanamide, N-[1-[1-(4-chloro-2-fluorophenyl)-2-(2-chlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-4-piperidinyl]-2-methyl- (CA INDEX NAME)



RN 960320-92-7 CAPLUS

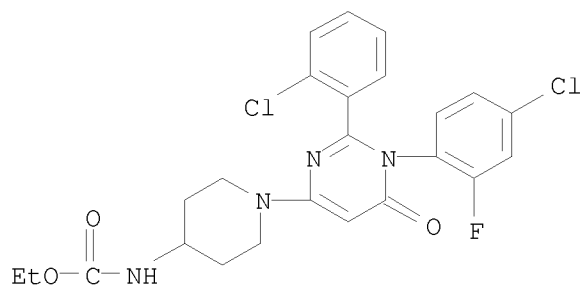
CN Urea, N'-[1-[1-(4-chloro-2-fluorophenyl)-2-(2-chlorophenyl)-1,6-dihydro-6-

oxo-4-pyrimidinyl]-4-piperidinyl]-N,N-dimethyl- (CA INDEX NAME)



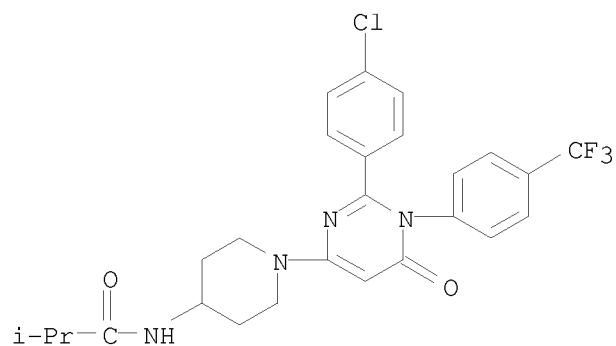
RN 960320-93-8 CAPLUS

CN Carbamic acid, N-[1-[1-(4-chloro-2-fluorophenyl)-2-(2-chlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-4-piperidinyl]-, ethyl ester (CA INDEX NAME)



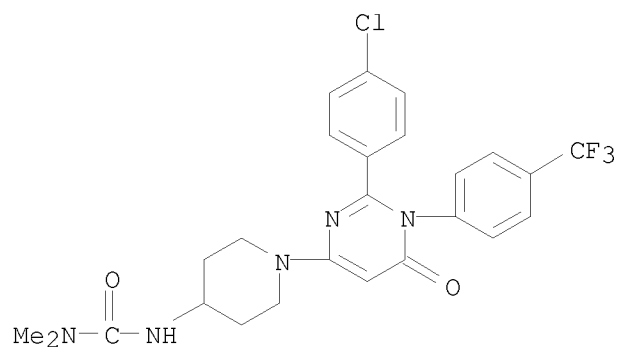
RN 960320-94-9 CAPLUS

CN Propanamide, N-[1-[2-(4-chlorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-2-methyl- (CA INDEX NAME)



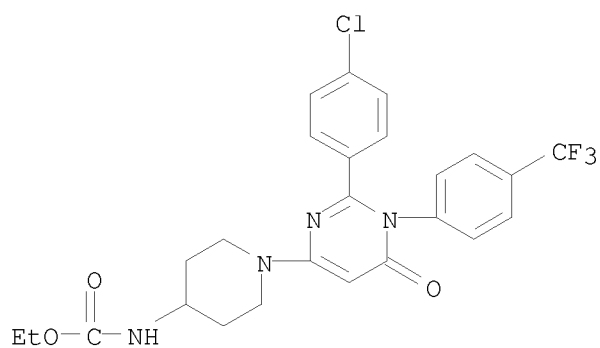
RN 960320-95-0 CAPLUS

CN Urea, N'-[1-[2-(4-chlorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-N,N-dimethyl- (CA INDEX NAME)



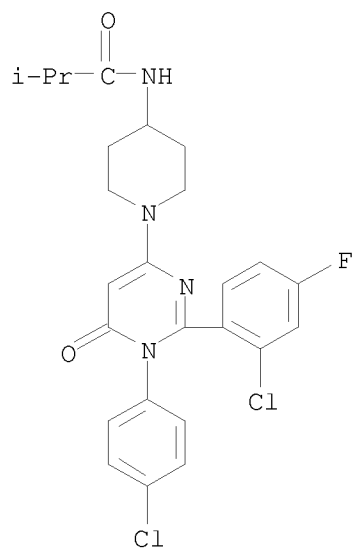
RN 960320-96-1 CAPLUS

CN Carbamic acid, N-[1-[2-(4-chlorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-, ethyl ester (CA INDEX NAME)



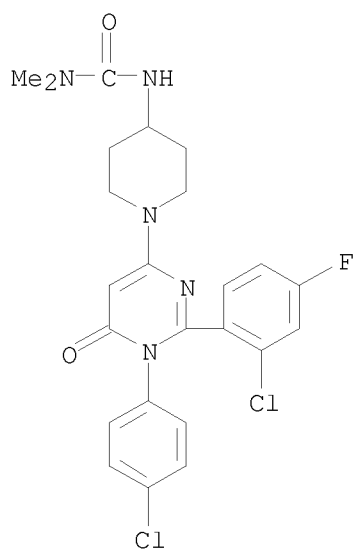
RN 960320-97-2 CAPLUS

CN Propanamide, N-[1-[2-(2-chloro-4-fluorophenyl)-1-(4-chlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-4-piperidinyl]-2-methyl- (CA INDEX NAME)



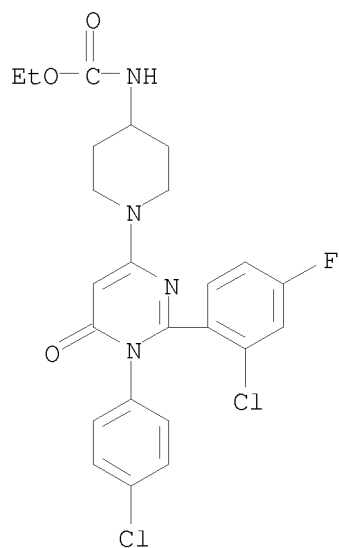
RN 960320-98-3 CAPLUS

CN Urea, N'-[1-[2-(2-chloro-4-fluorophenyl)-1-(4-chlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-4-piperidinyl]-N,N-dimethyl- (CA INDEX NAME)



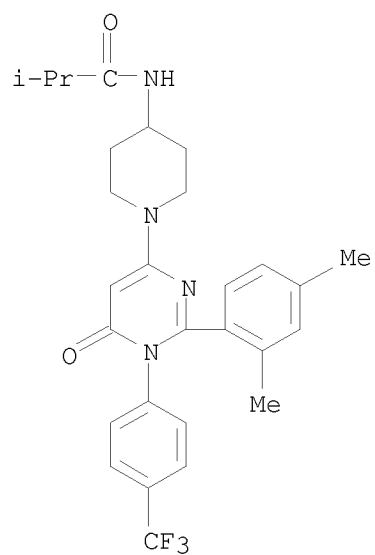
RN 960320-99-4 CAPLUS

CN Carbamic acid, N-[1-[2-(2-chloro-4-fluorophenyl)-1-(4-chlorophenyl)-1,6-dihydro-6-oxo-4-pyrimidinyl]-4-piperidinyl]-, ethyl ester (CA INDEX NAME)



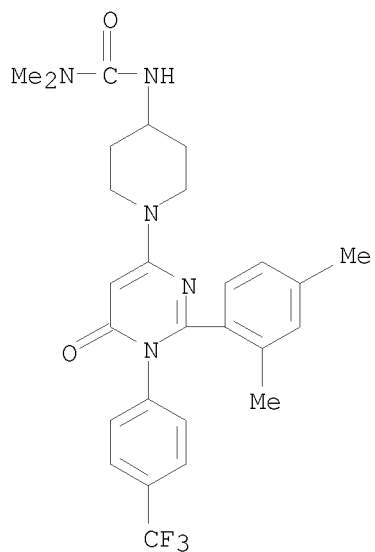
RN 960321-00-0 CAPLUS

CN Propanamide, N-[1-[2-(2,4-dimethylphenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-2-methyl- (CA INDEX NAME)



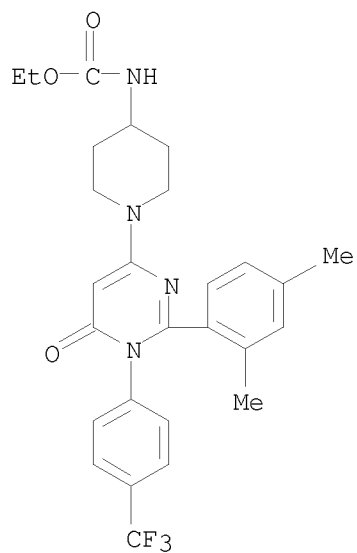
RN 960321-01-1 CAPLUS

CN Urea, N'-[1-[2-(2,4-dimethylphenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-N,N-dimethyl- (CA INDEX NAME)



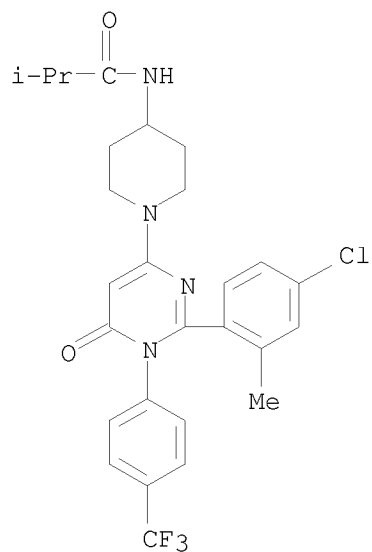
RN 960321-02-2 CAPLUS

CN Carbamic acid, N-[1-[2-(2,4-dimethylphenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-, ethyl ester (CA INDEX NAME)



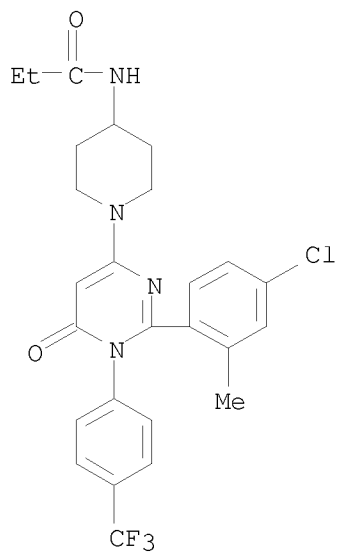
RN 960321-03-3 CAPLUS

CN Propanamide, N-[1-[2-(4-chloro-2-methylphenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-2-methyl-4-piperidinyl]-, ethyl ester (CA INDEX NAME)



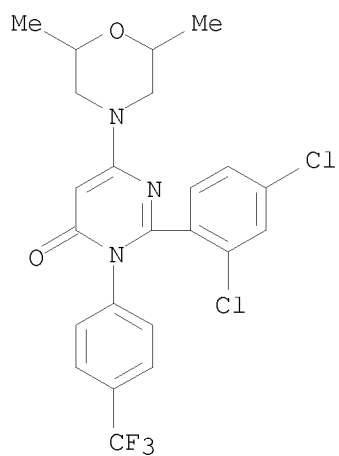
RN 960321-04-4 CAPLUS

CN Propanamide, N-[1-[2-(4-chloro-2-methylphenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]- (CA INDEX NAME)



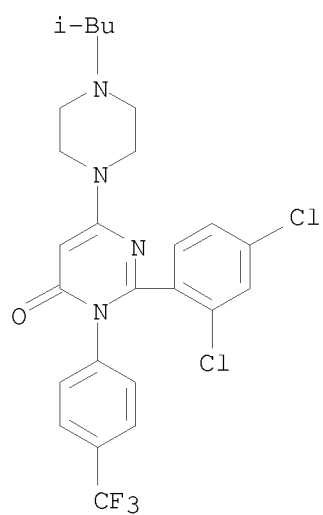
RN 960321-05-5 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2,4-dichlorophenyl)-6-(2,6-dimethyl-4-morpholinyl)-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



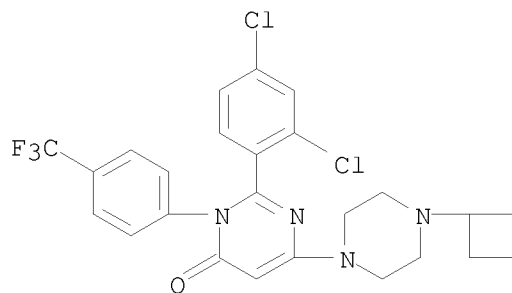
RN 960321-06-6 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2,4-dichlorophenyl)-6-[4-(2-methylpropyl)-1-piperazinyl]-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



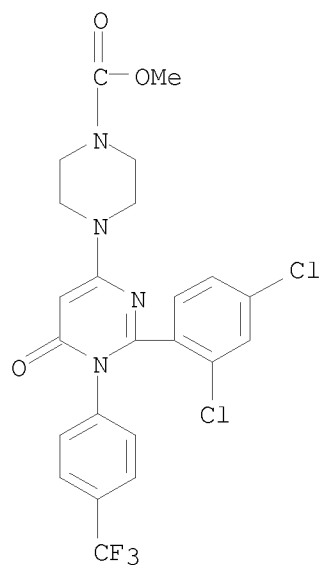
RN 960321-07-7 CAPLUS

CN 4(3H)-Pyrimidinone, 6-(4-cyclobutyl-1-piperazinyl)-2-(2,4-dichlorophenyl)-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



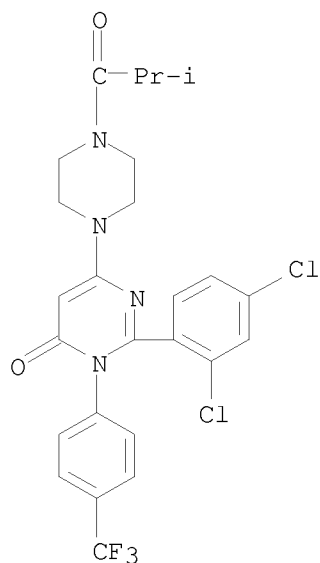
RN 960321-08-8 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[2-(2,4-dichlorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-, methyl ester (CA INDEX NAME)



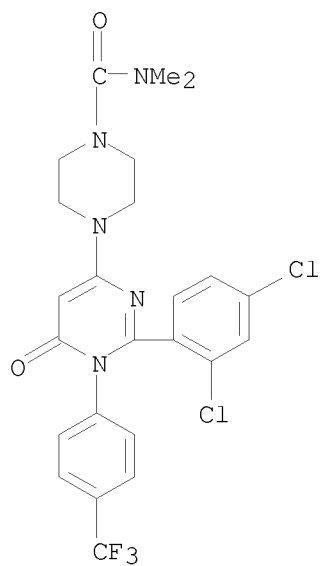
RN 960321-09-9 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2,4-dichlorophenyl)-6-[4-(2-methyl-1-oxopropyl)-1-piperazinyl]-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



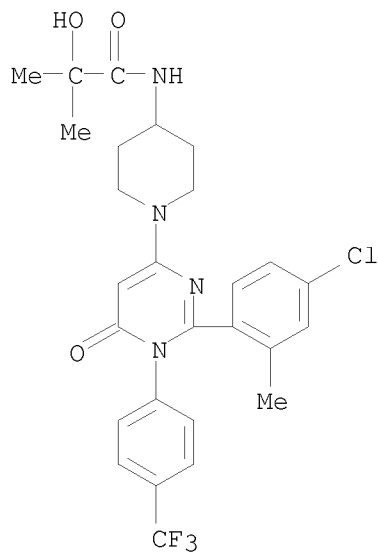
RN 960321-10-2 CAPLUS

CN 1-Piperazinecarboxamide, 4-[2-(2,4-dichlorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-N,N-dimethyl- (CA INDEX NAME)



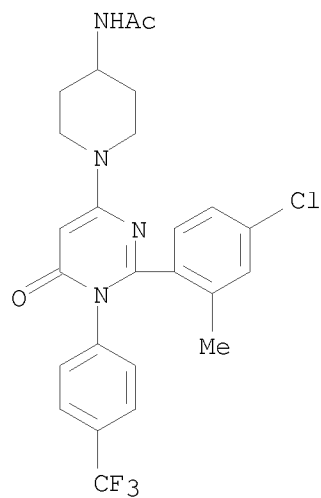
RN 960321-11-3 CAPLUS

CN Propanamide, N-[1-[2-(4-chloro-2-methylphenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidiny]-2-hydroxy-2-methyl- (CA INDEX NAME)



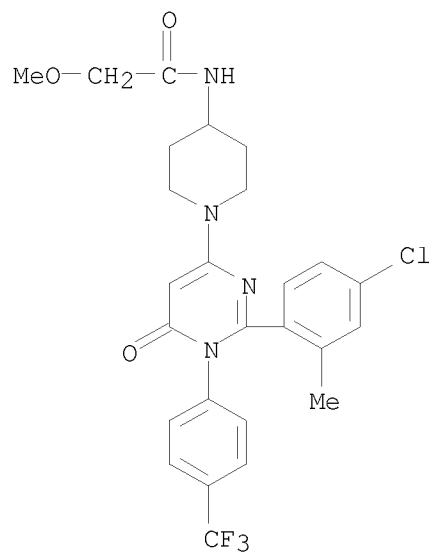
RN 960321-12-4 CAPLUS

CN Acetamide, N-[1-[2-(4-chloro-2-methylphenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]- (CA INDEX NAME)



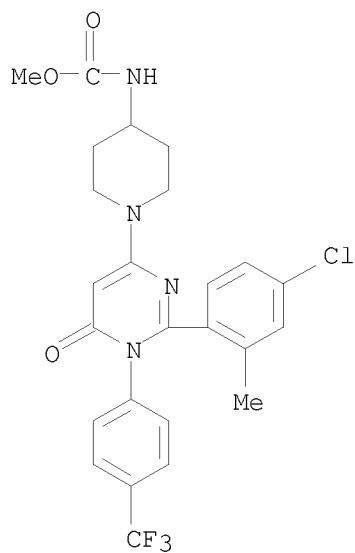
RN 960321-13-5 CAPLUS

CN Acetamide, N-[1-[2-(4-chloro-2-methylphenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-2-methoxy- (CA INDEX NAME)



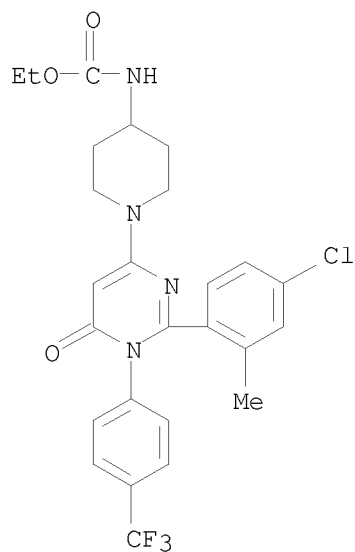
RN 960321-14-6 CAPLUS

CN Carbamic acid, N-[1-[2-(4-chloro-2-methylphenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-, methyl ester (CA INDEX NAME)



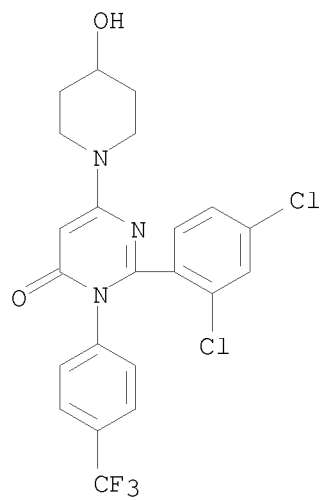
RN 960321-15-7 CAPLUS

CN Carbamic acid, N-[1-[2-(4-chloro-2-methylphenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-, ethyl ester (CA INDEX NAME)



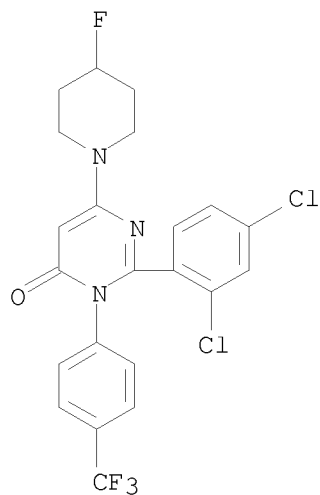
RN 960321-16-8 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2,4-dichlorophenyl)-6-(4-hydroxy-1-piperidinyl)-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



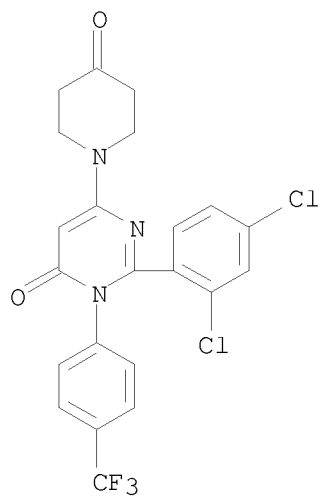
RN 960321-17-9 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2,4-dichlorophenyl)-6-(4-fluoro-1-piperidinyl)-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



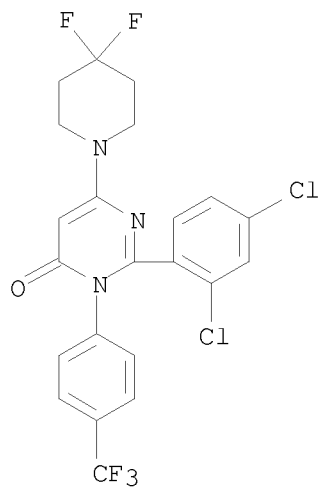
RN 960321-18-0 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2,4-dichlorophenyl)-6-(4-oxo-1-piperidinyl)-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



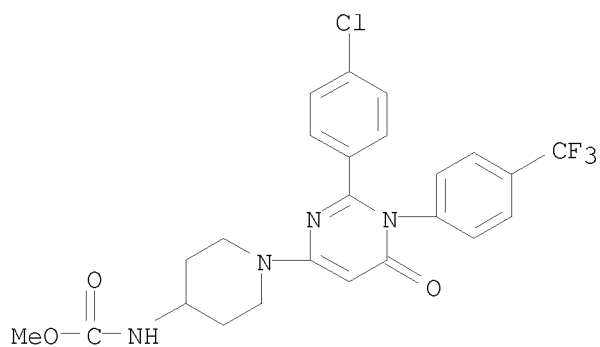
RN 960321-22-6 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2,4-dichlorophenyl)-6-(4,4-difluoro-1-piperidinyl)-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



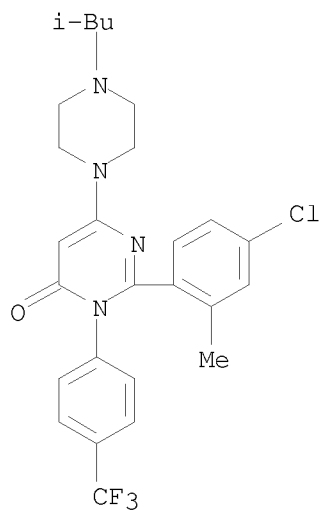
RN 960321-26-0 CAPLUS

CN Carbamic acid, N-[1-[2-(4-chlorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-, methyl ester (CA INDEX NAME)



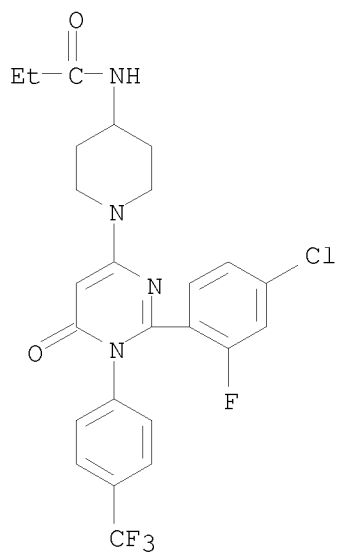
RN 960321-27-1 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(4-chloro-2-methylphenyl)-6-[4-(2-methylpropyl)-1-piperazinyl]-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



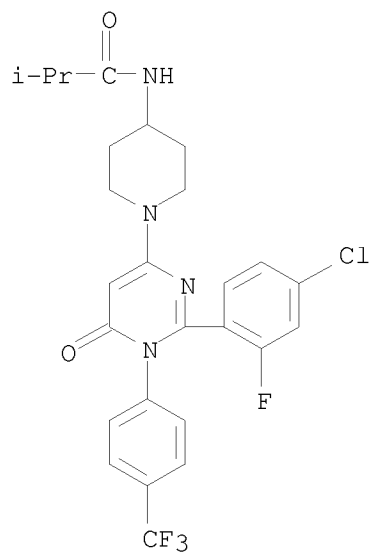
RN 960321-31-7 CAPLUS

CN Propanamide, N-[1-[2-(4-chloro-2-fluorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]- (CA INDEX NAME)



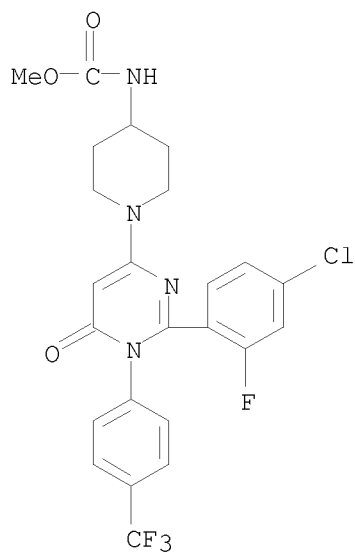
RN 960321-32-8 CAPLUS

CN Propanamide, N-[1-[2-(4-chloro-2-fluorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-2-methyl- (CA INDEX NAME)



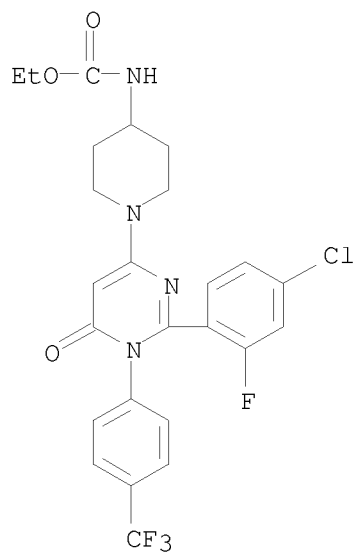
RN 960321-33-9 CAPLUS

CN Carbamic acid, N-[1-[2-(4-chloro-2-fluorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-, methyl ester (CA INDEX NAME)



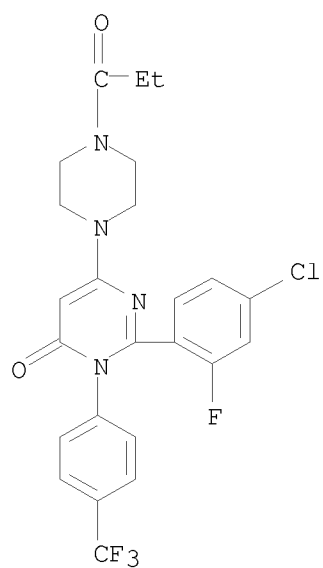
RN 960321-34-0 CAPLUS

CN Carbamic acid, N-[1-[2-(4-chloro-2-fluorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-, ethyl ester (CA INDEX NAME)



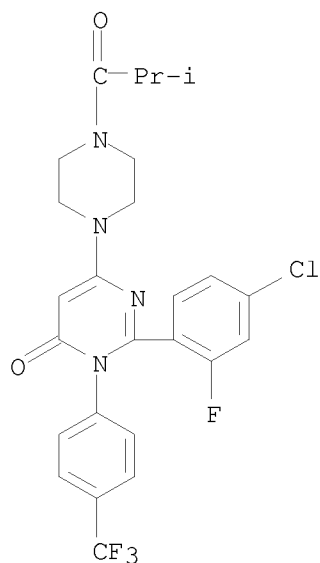
RN 960321-39-5 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(4-chloro-2-fluorophenyl)-6-[4-(1-oxopropyl)-1-piperazinyl]-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



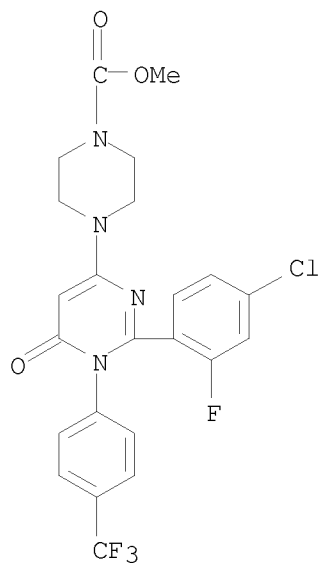
RN 960321-40-8 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(4-chloro-2-fluorophenyl)-6-[4-(2-methyl-1-oxopropyl)-1-piperazinyl]-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



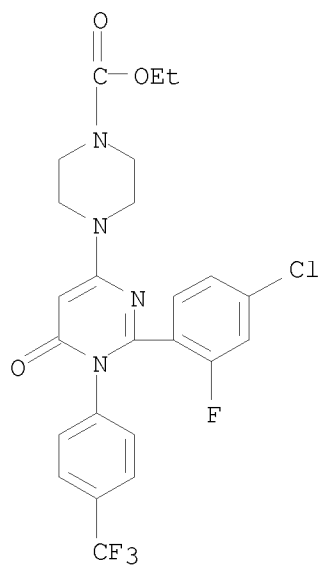
RN 960321-41-9 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[2-(4-chloro-2-fluorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-, methyl ester (CA INDEX NAME)



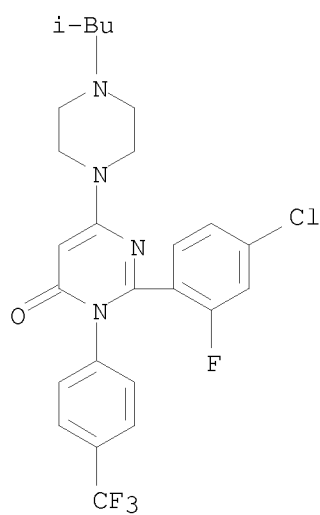
RN 960321-42-0 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[2-(4-chloro-2-fluorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-, ethyl ester (CA INDEX NAME)



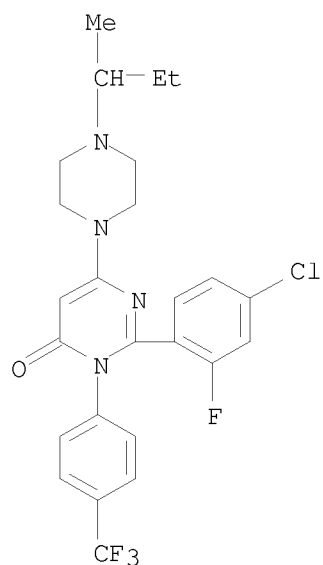
RN 960321-43-1 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(4-chloro-2-fluorophenyl)-6-[4-(2-methylpropyl)-1-piperazinyl]-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



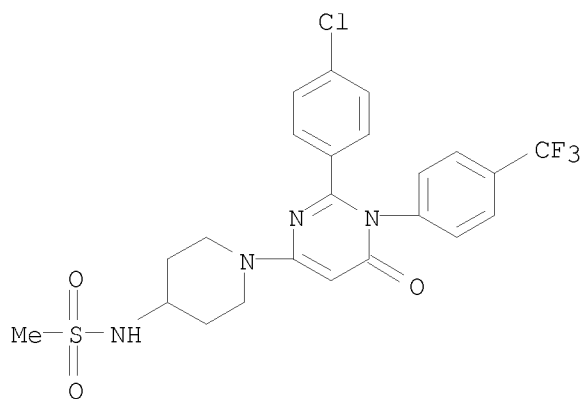
RN 960321-44-2 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(4-chloro-2-fluorophenyl)-6-[4-(1-methylpropyl)-1-piperazinyl]-3-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



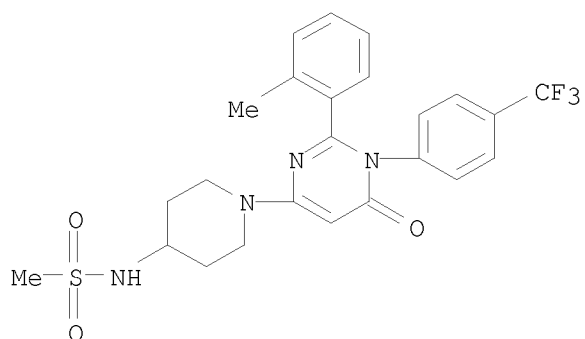
RN 960321-46-4 CAPLUS

CN Methanesulfonamide, N-[1-[2-(4-chlorophenyl)-1,6-dihydro-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]- (CA INDEX NAME)



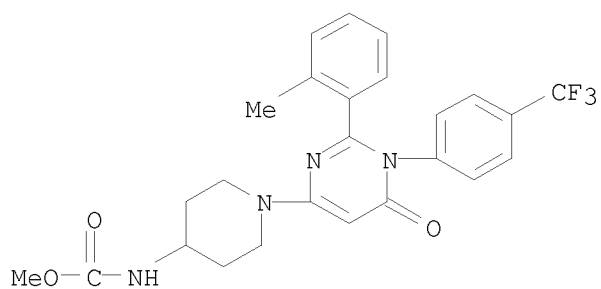
RN 960321-47-5 CAPLUS

CN Methanesulfonamide, N-[1-[1,6-dihydro-2-(2-methylphenyl)-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]- (CA INDEX NAME)



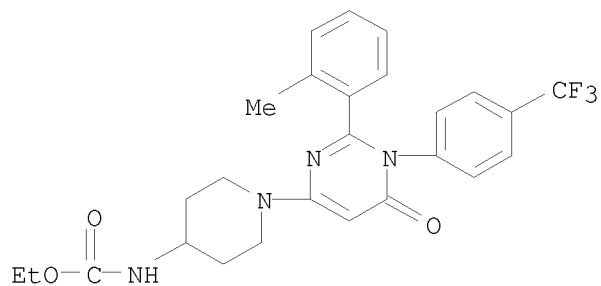
RN 960321-52-2 CAPLUS

CN Carbamic acid, N-[1-[1,6-dihydro-2-(2-methylphenyl)-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-, methyl ester (CA INDEX NAME)



RN 960321-53-3 CAPLUS

CN Carbamic acid, N-[1-[1,6-dihydro-2-(2-methylphenyl)-6-oxo-1-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]-4-piperidinyl]-, ethyl ester (CA INDEX NAME)



L17 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 AN 2007:329344 CAPLUS
 DN 146:337904
 TI Preparation of pyrimidine carboxamides as inhibitors of cytokines and COX-2
 IN Tadiparthi, Ravikumar; Aggarwal, Pawan; Parameswaran, Venkatesan; Thirunavukkarasu, Sappanimuthu; Barik, Rajib; Rajagopal, Sriram; Reddy, Gaddam Om
 PA Orchid Research Laboratories Limited, India
 SO PCT Int. Appl., 75pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2007031829	A2	20070322	WO 2006-IB2461	20060907
	WO 2007031829	A3	20071108		
	W:		AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW		
	RW:		AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA		
	IN 2005CH01302	A	20070727	IN 2005-CH1302	20050915
	AU 2006290465	A1	20070322	AU 2006-290465	20060907
	US 20070072876	A1	20070329	US 2006-516549	20060907
	EP 1931642	A2	20080618	EP 2006-795441	20060907
	R:		AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR		
PRAI	IN 2005-CH1302	A	20050915		
	WO 2006-IB2461	W	20060907		
OS	MARPAT 146:337904				
AB	Title compds. represented by the formula I [wherein R = H, halo, amino, etc.; R1, R3 = independently H, SR6 or SOR7; R2, R4 = independently H, hydroxy, halo, etc.; R5 = H, hydroxy, azido, etc.; and their derivs., analogs, tautomers, stereoisomers, polymorphs, hydrates, solvates, pharmaceutically acceptable salts and compns. thereof] were prepared as Cyclooxygenase-2 (COX-2) inhibitors. For example, II was provided in a multi-step synthesis starting from 5-cyano-1-(4-methylphenyl)-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo-1,6-dihydropyrimidine. I were tested in vitro evaluation of COX-2 inhibition activity in human whole blood assay, COX-1 and COX-2 enzyme based assay, in vitro measurement of tumor necrosis factor alpha (TNF- α), and etc. Thus, I and their pharmaceutical compns. are useful for the prophylaxis or treatment of a pain disorder, inflammation, and immunol. diseases in a mammal, which are mediated by TNF- α , IL (1 β , 1,6,8,12) and COX-2 activity.				
IT	613663-83-5, 5-Cyano-1-(4-methylphenyl)-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo-1,6-dihydropyrimidine 812691-93-3, 5-Cyano-1-(3,4-dimethylphenyl)-4-(methylthio)-2-[4-(methylthio)phenyl]-6-				

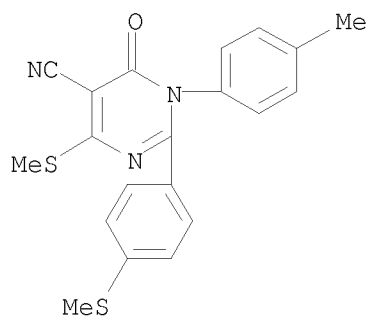
oxo-1,6-dihydropyrimidine

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of pyrimidine carboxamides as inhibitors of cytokines and COX-2)

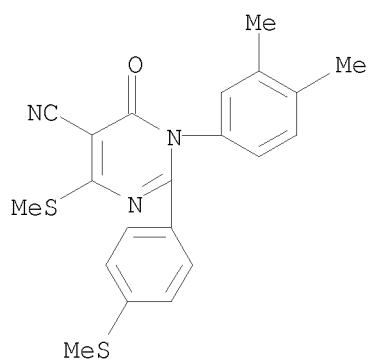
RN 613663-83-5 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1,6-dihydro-1-(4-methylphenyl)-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



RN 812691-93-3 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1-(3,4-dimethylphenyl)-1,6-dihydro-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



L17 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

AN 2007:300062 CAPLUS

DN 147:427365

TI Pyrazolopyrimidinone derivatives for the treatment of inflammation and immunological diseases, their preparation, pharmaceutical compositions, and use in therapy

IN Agarwal, Shiv Kumar; Ravikumar, Tadiparthi; Aggarwal, Pawan; Shivakumar, Savithiri

PA Orchid Chemicals & Pharmaceuticals Ltd., India

SO Indian Pat. Appl., 23pp.

CODEN: INXXBQ

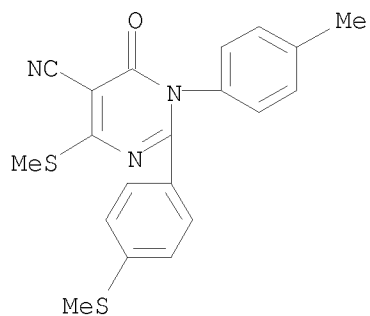
DT Patent

LA English

FAN.CNT 1

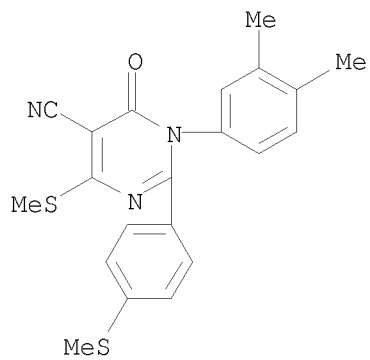
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	IN 2004CH00316	A	20060113	IN 2004-CH316	20040406
PRAI	IN 2004-CH316		20040406		
OS	CASREACT 147:427365; MARPAT 147:427365				
AB	The invention relates to pyrazolo[3,4-d]pyrimidin-4-ones of general formula I, which are useful for the treatment of inflammation and immunol. diseases. In compds. I, Ar1 and Ar2 are independently selected from (un)substituted aryl, (un)substituted heteroaryl, and (un)substituted heterocyclyl; R1 is H, halo, OH, NH2, formyl, alkylamino, arylamino, acylamino, sulfonylamino, substituted C1-6 alkyl, (un)substituted acyl, (un)substituted aryl, (un)substituted aralkyl, (un)substituted heteroaryl, (un)substituted heteroarylalkyl, or (un)substituted heterocyclyl; and R2 is selected from H, halo, OH, nitro, azido, alkyl, (un)substituted alkoxy, (un)substituted aryloxy, (un)substituted aralkyl, (un)substituted heteroaryl, (un)substituted acyl, (un)substituted acyloxy, (un)substituted (di)alkylamino, (un)substituted heterocyclyl, etc.; including tautomers, stereoisomers, polymorphs, hydrates, solvates, and salts thereof. The invention also relates to the preparation of I, pharmaceutical compns. comprising a compound I, as well as to the use of the compns. for the treatment of inflammation and immunol. diseases. Substitution of pyrimidinone II with hydrazine hydrate followed by intramol. heterocyclization gave pyrazolopyrimidinone III. The compds. of the invention, e.g., III, are inhibitors of cyclooxygenase-2 (no data).				
IT	613663-83-5, 5-Cyano-1-(4-methylphenyl)-4-methylthio-2-(4-(methylthio)phenyl)-1,6-dihydropyrimidin-6-one 812691-93-3, 5-Cyano-1-(3,4-dimethylphenyl)-4-methylthio-2-(4-(methylthio)phenyl)-1,6-dihydropyrimidin-6-one				
RL	RCT (Reactant); RACT (Reactant or reagent) (starting material; preparation of pyrazolopyrimidinone derivs. for the treatment of inflammation and immunol. diseases)				
RN	613663-83-5 CAPLUS				
CN	5-Pyrimidinecarbonitrile, 1,6-dihydro-1-(4-methylphenyl)-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)				

10/582,826



RN 812691-93-3 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1-(3,4-dimethylphenyl)-1,6-dihydro-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



L17 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

AN 2007:14078 CAPLUS

DN 146:121982

TI Preparation of pyrazolopyrimidinone derivatives as inhibitors of production of cytokines for treatment of inflammation, cancer, etc.

IN Tadiparthi, Ravikumar; Pushpan, Simi; Rajagopal, Sriram; Barik, Rajib

PA Orchid Research Laboratories Limited, India

SO PCT Int. Appl., 46pp.

CODEN: PIXXD2

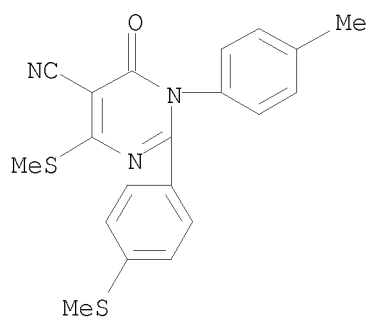
DT Patent

LA English

FAN.CNT 1

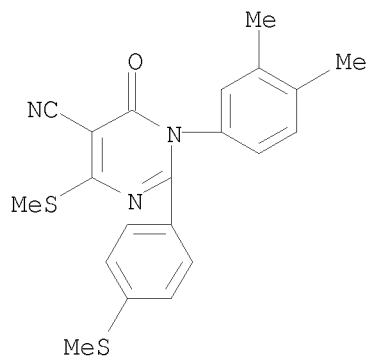
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2007000655	A2	20070104	WO 2006-IB1791	20060628
	WO 2007000655	A3	20070322		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
	RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	IN 2005CH00813	A	20080509	IN 2005-CH813	20050628
	EP 1896476	A2	20080312	EP 2006-765607	20060628
	R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR			
	JP 2008543968	T	20081204	JP 2008-519006	20060628
PRAI	IN 2005-CH813	A	20050628		
	WO 2006-IB1791	W	20060628		
OS	MARPAT 146:121982				
AB	The title compds. I [Ar1, Ar2 = (un)substituted aryl, heteroaryl, heterocyclyl; R1 = H, hydroxyl, halo, etc.; R2 = H, hydroxy, nitro, etc.] are prepared Thus, 3-amino-5-(4-methylphenyl)-6-[4-(methylthio)phenyl]-1,5-dihydro-4H-pyrazolo[3,4-d]pyrimidin-4-one was prepared by from hydrazine hydrate and 5-cyano-1-(4-methylphenyl)-4-methylthio-2-(4-methylthiophenyl)-1,6-dihydropyrimidin-6-one. In an in vitro assay using human peripheral blood mononuclear cells and lipopolysaccharide, compds. of this invention at 10 μ M gave 29.8-87.8% inhibition of TNF- α production				
IT	613663-83-5 812691-93-3				
	RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of pyrazolopyrimidinone derivs. as inhibitors of production of cytokines for treatment of inflammation and cancer)				
RN	613663-83-5 CAPLUS				
CN	5-Pyrimidinecarbonitrile, 1,6-dihydro-1-(4-methylphenyl)-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)				

10/582,826



RN 812691-93-3 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1-(3,4-dimethylphenyl)-1,6-dihydro-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



L17 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 AN 2006:1283525 CAPLUS
 DN 146:45537
 TI Preparation of pyrimidinedione derivatives for treating inflammatory diseases
 IN Tadiparthi, Ravikumar; Aggarwal, Pawan; Reddy, Gaddam Om; Parameswaran, Venkatesan; Rajagopal, Iram, Sr.; Raghuveeraswaminathan, Sankaranarayanan
 PA Orchid Research Laboratories Limited, India
 SO PCT Int. Appl., 42pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2006129181	A2	20061207	WO 2006-IB1448	20060602
	WO 2006129181	A3	20071227		
	W:				
	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW:				
	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				

IN 2005CH00682 A 20070727 IN 2005-CH682 20050603

PRAI IN 2005-CH682 A 20050603

OS CASREACT 146:45537; MARPAT 146:45537

AB Title compds. represented by the formula I [wherein X = O or S; ring A, B = (hetero)aryl; R = H, OH, amino or (halo)alkyl; R1, R3 = independently H, SR5 or SOPr6; R2, R4 = independently H, halo, OH, NO2, etc.; R5 = H, alkyl(halide), aryl or alkylester; R6 = amino, OH, halo, etc.; Y = -C(=NH)R8 or -C(=NR9)R8; R8, R9 = independently H, amino, azido, etc.; m, n = 0-4; p = 1 or 2], useful for treating inflammatory diseases mediated by cytokines such as TNF- α , IL-1, IL-6, IL-8 and IL-12, were prepared E.g., reaction of 5-cyano-1-(4-methylphenyl)-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo-1,6-dihydropyrimidine with methylamine gave II, which showed TNF- α inhibition with IC50 value of 2.6 μ M.

Pharmaceutical composition comprising the compound I is claimed.

IT 916451-81-5P, N-Methyl-1-(4-methylphenyl)-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo-1,6-dihydropyrimidine-5-carboximidamide
 916451-82-6P, N-Methyl-1-(3,4-dimethylphenyl)-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo-1,6-dihydropyrimidine-5-carboximidamide
 916451-83-7P, N-Methyl-1-(4-isopropylphenyl)-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo-1,6-dihydropyrimidine-5-carboximidamide
 916451-84-8P, N-Methyl-1-(3,4,5-trimethoxyphenyl)-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo-1,6-dihydropyrimidine-5-carboximidamide
 916451-85-9P 916451-88-2P 916451-89-3P,
 1-(4-Chlorophenyl)-N-methyl-2-[4-(methylthio)phenyl]-6-oxo-1,6-dihydropyrimidine-5-carboximidamide 916451-90-6P
 916451-92-8P 916451-93-9P 916451-94-0P,
 2-(4-Methoxyphenyl)-N-methyl-4-(methylthio)-1-[4-(methylthio)phenyl]-6-oxo-1,6-dihydropyrimidine-5-carboximidamide 916452-00-1P

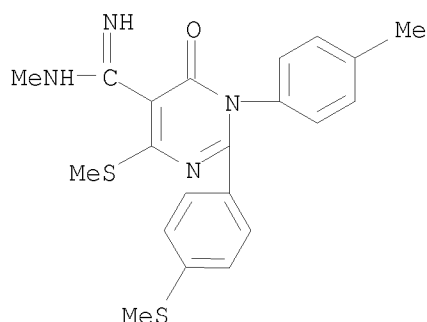
916452-01-2P 916452-02-3P,
 2-[4-(Aminosulfonyl)phenyl]-N-methyl-4-(methylthio)-6-oxo-1-phenyl-1,6-dihydropyrimidine-5-carboximidamide 916452-03-4P,
 2-[4-(Aminosulfonyl)phenyl]-N-methyl-4-(methylthio)-6-oxo-1-(4-methylphenyl)-1,6-dihydropyrimidine-5-carboximidamide 916452-04-5P,
 , 2-[4-(Aminosulfonyl)phenyl]-N-methyl-4-(methylthio)-6-oxo-1-(3,4-dimethylphenyl)-1,6-dihydropyrimidine-5-carboximidamide
 916452-05-6P, 2-[4-(Aminosulfonyl)phenyl]-N-methyl-4-(methylthio)-6-oxo-1-(4-fluorophenyl)-1,6-dihydropyrimidine-5-carboximidamide
 916452-07-8P, 1-[4-(Aminosulfonyl)phenyl]-N-methyl-4-(methylthio)-6-oxo-2-(4-methylphenyl)-1,6-dihydropyrimidine-5-carboximidamide
 916452-08-9P, 1-[4-(Aminosulfonyl)phenyl]-N-methyl-4-(methylthio)-6-oxo-2-(3,4-dimethylphenyl)-1,6-dihydropyrimidine-5-carboximidamide
 916452-09-0P, 1-[4-(Aminosulfonyl)phenyl]-N-methyl-4-(methylthio)-6-oxo-2-(4-isopropylphenyl)-1,6-dihydropyrimidine-5-carboximidamide
 916452-15-8P, 2-(4-Methylthiophenyl)-N-methyl-4-(1-methylhydrazino)-1-(4-methylphenyl)-6-oxo-1,6-dihydropyrimidine-5-carboximidamide 916452-16-9P 916452-17-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrimidinedione derivs. for treating inflammatory diseases)

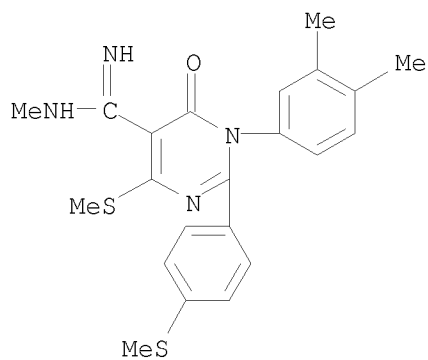
RN 916451-81-5 CAPLUS

CN 5-Pyrimidinecarboximidamide, 1,6-dihydro-N-methyl-1-(4-methylphenyl)-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



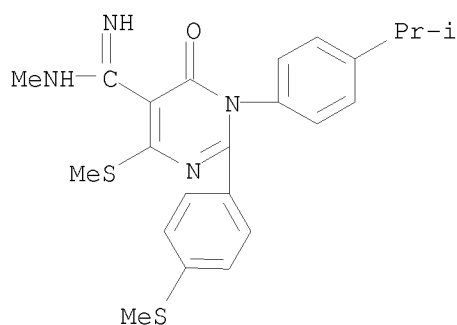
RN 916451-82-6 CAPLUS

CN 5-Pyrimidinecarboximidamide, 1-(3,4-dimethylphenyl)-1,6-dihydro-N-methyl-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



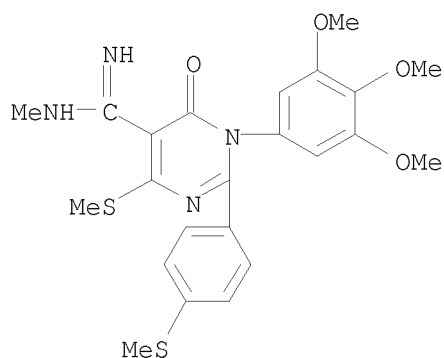
RN 916451-83-7 CAPLUS

CN 5-Pyrimidinecarboximidamide, 1,6-dihydro-N-methyl-1-[4-(1-methylethyl)phenyl]-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



RN 916451-84-8 CAPLUS

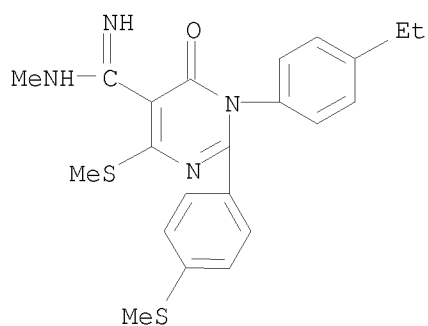
CN 5-Pyrimidinecarboximidamide, 1,6-dihydro-N-methyl-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo-1-(3,4,5-trimethoxyphenyl)- (CA INDEX NAME)



RN 916451-85-9 CAPLUS

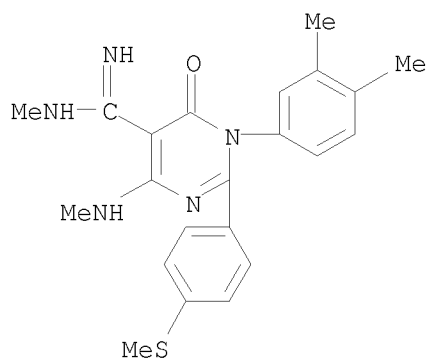
CN 5-Pyrimidinecarboximidamide, 1-(4-ethylphenyl)-1,6-dihydro-N-methyl-4-

(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



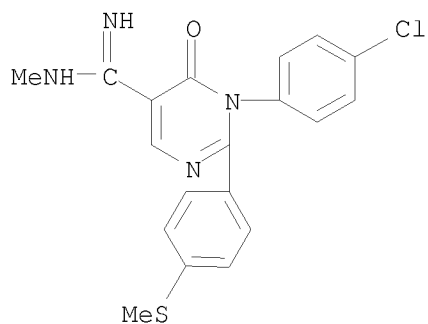
RN 916451-88-2 CAPLUS

CN 5-Pyrimidinecarboximidamide, 1-(3,4-dimethylphenyl)-1,6-dihydro-N-methyl-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



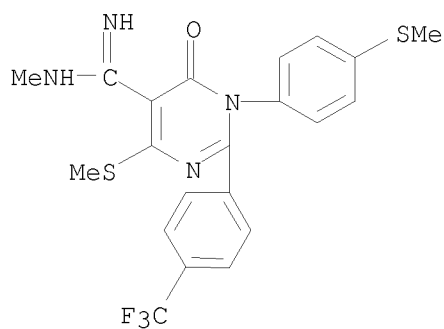
RN 916451-89-3 CAPLUS

CN 5-Pyrimidinecarboximidamide, 1-(4-chlorophenyl)-1,6-dihydro-N-methyl-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



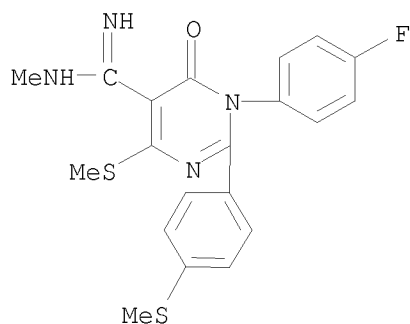
RN 916451-90-6 CAPLUS

CN 5-Pyrimidinecarboximidamide, 1,6-dihydro-N-methyl-4-(methylthio)-1-[4-(methylthio)phenyl]-6-oxo-2-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



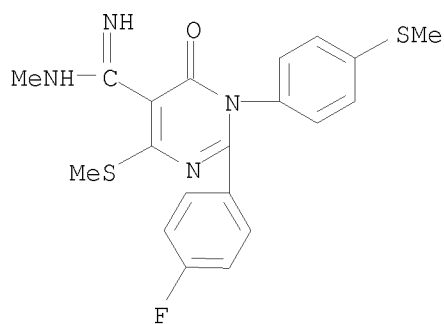
RN 916451-92-8 CAPLUS

CN 5-Pyrimidinecarboximidamide, 1-(4-fluorophenyl)-1,6-dihydro-N-methyl-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



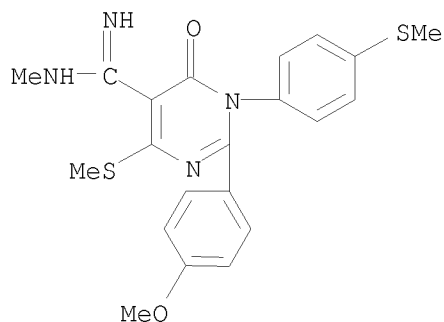
RN 916451-93-9 CAPLUS

CN 5-Pyrimidinecarboximidamide, 2-(4-fluorophenyl)-1,6-dihydro-N-methyl-4-(methylthio)-1-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



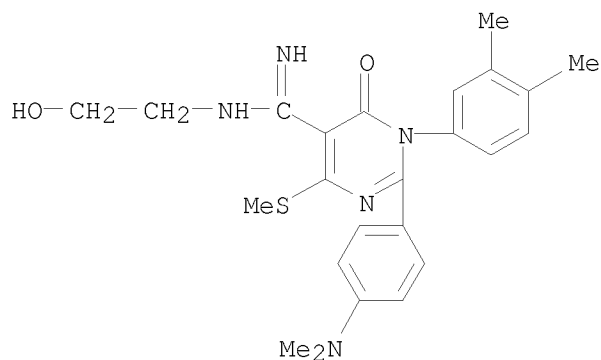
RN 916451-94-0 CAPLUS

CN 5-Pyrimidinecarboximidamide, 1,6-dihydro-2-(4-methoxyphenyl)-N-methyl-4-(methylthio)-1-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



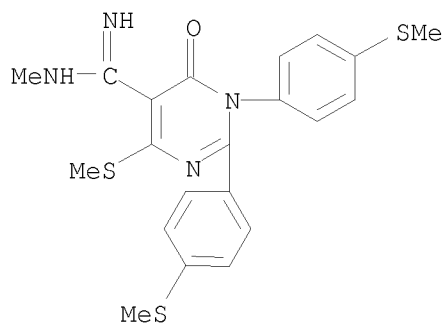
RN 916452-00-1 CAPLUS

CN 5-Pyrimidinecarboximidamide, 2-[4-(dimethylamino)phenyl]-1-(3,4-dimethylphenyl)-1,6-dihydro-N-(2-hydroxyethyl)-4-(methylthio)-6-oxo- (CA INDEX NAME)



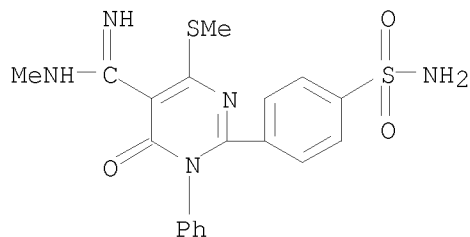
RN 916452-01-2 CAPLUS

CN 5-Pyrimidinecarboximidamide, 1,6-dihydro-N-methyl-4-(methylthio)-1,2-bis[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



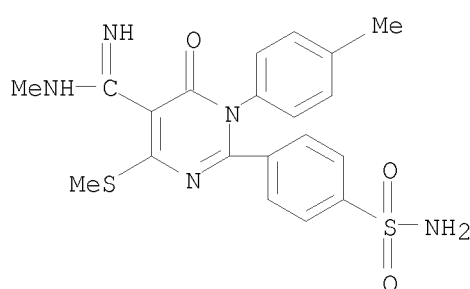
RN 916452-02-3 CAPLUS

CN 5-Pyrimidinecarboximidamide, 2-[4-(aminosulfonyl)phenyl]-1,6-dihydro-N-methyl-4-(methylthio)-6-oxo-1-phenyl- (CA INDEX NAME)



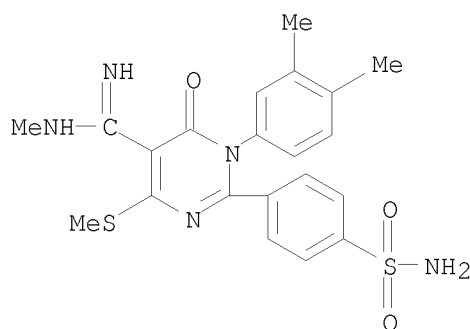
RN 916452-03-4 CAPLUS

CN 5-Pyrimidinecarboximidamide, 2-[4-(aminosulfonyl)phenyl]-1,6-dihydro-N-methyl-1-(4-methylphenyl)-4-(methylthio)-6-oxo- (CA INDEX NAME)



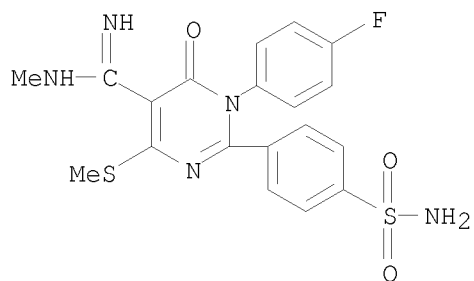
RN 916452-04-5 CAPLUS

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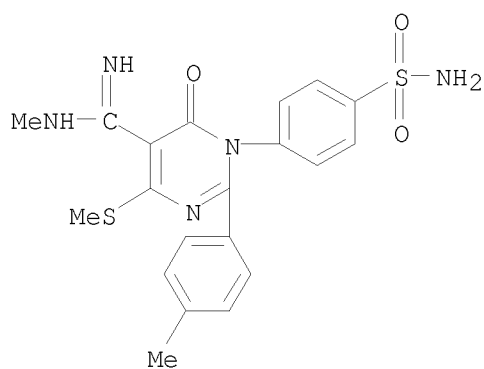
RN 916452-05-6 CAPLUS

CN 5-Pyrimidinecarboximidamide, 2-[4-(aminosulfonyl)phenyl]-1-(4-fluorophenyl)-1,6-dihydro-N-methyl-4-(methylthio)-6-oxo- (CA INDEX NAME)



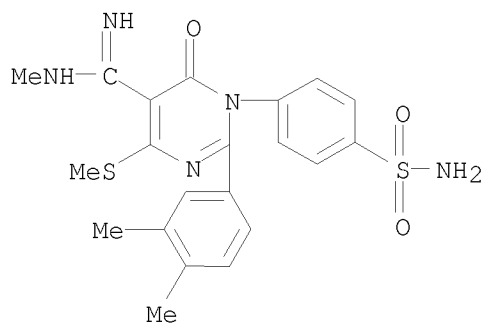
RN 916452-07-8 CAPLUS

CN 5-Pyrimidinecarboximidamide, 1-[4-(aminosulfonyl)phenyl]-1,6-dihydro-N-methyl-2-(4-methylphenyl)-4-(methylthio)-6-oxo- (CA INDEX NAME)



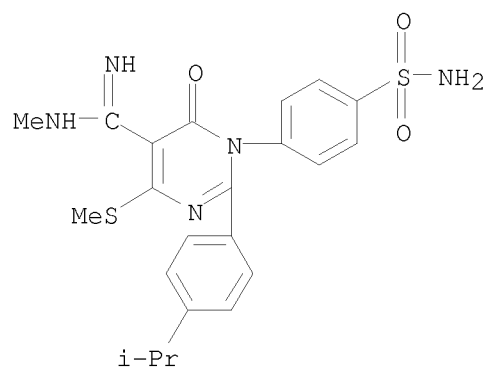
RN 916452-08-9 CAPLUS

CN 5-Pyrimidinecarboximidamide, 1-[4-(aminosulfonyl)phenyl]-2-(3,4-dimethylphenyl)-1,6-dihydro-N-methyl-4-(methylthio)-6-oxo- (CA INDEX NAME)



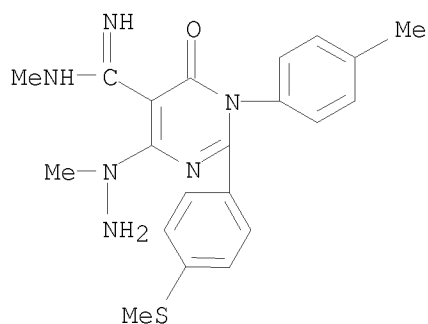
RN 916452-09-0 CAPLUS

CN 5-Pyrimidinecarboximidamide, 1-[4-(aminosulfonyl)phenyl]-1,6-dihydro-N-methyl-2-[4-(1-methylethyl)phenyl]-4-(methylthio)-6-oxo- (CA INDEX NAME)



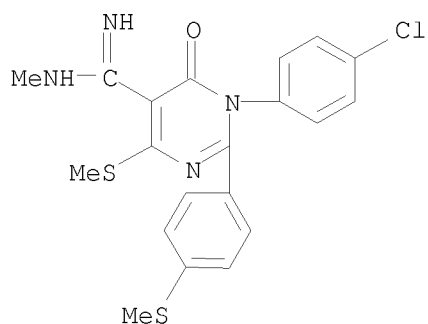
RN 916452-15-8 CAPLUS

CN 5-Pyrimidinecarboximidamide, 1,6-dihydro-N-methyl-4-(1-methylhydrazinyl)-1-(4-methylthiophenyl)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



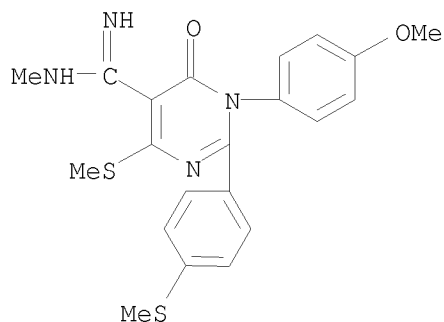
RN 916452-16-9 CAPLUS

CN 5-Pyrimidinecarboximidamide, 1-(4-chlorophenyl)-1,6-dihydro-N-methyl-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)

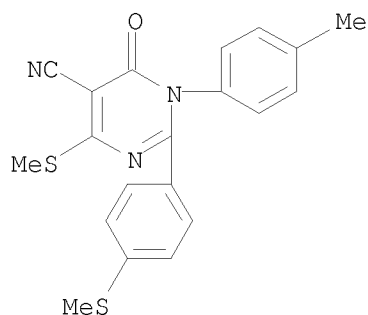


RN 916452-17-0 CAPLUS

CN 5-Pyrimidinecarboximidamide, 1,6-dihydro-1-(4-methoxyphenyl)-N-methyl-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)

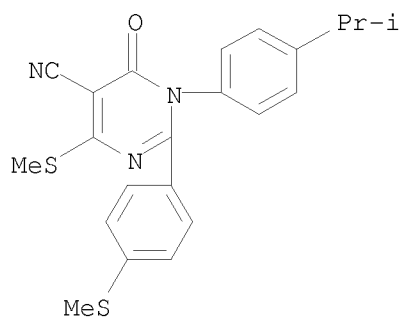


IT 613663-83-5, 5-Cyano-1-(4-methylphenyl)-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo-1,6-dihydropyrimidine 812691-92-2, 5-Cyano-1-(4-isopropylphenyl)-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo-1,6-dihydropyrimidine 812691-93-3, 5-Cyano-1-(3,4-dimethylphenyl)-4-(methylthio)-6-oxo-2-(pyridin-3-yl)-1,6-dihydropyrimidine 812691-96-6, 5-Cyano-1-(3,4,5-trimethoxyphenyl)-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo-1,6-dihydropyrimidine
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of pyrimidinedione derivs. for treating inflammatory diseases)
 RN 613663-83-5 CAPLUS
 CN 5-Pyrimidinecarbonitrile, 1,6-dihydro-1-(4-methylphenyl)-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



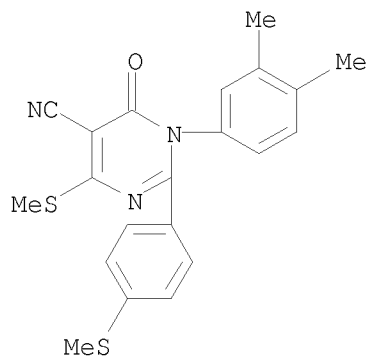
RN 812691-92-2 CAPLUS
 CN 5-Pyrimidinecarbonitrile, 1,6-dihydro-1-[4-(1-methylethyl)phenyl]-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)

10/582,826



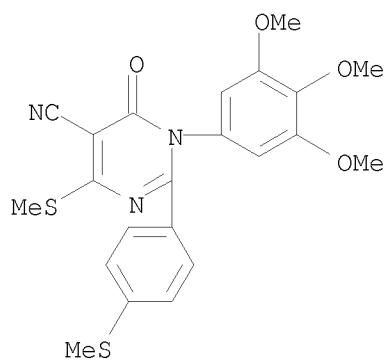
RN 812691-93-3 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1-(3,4-dimethylphenyl)-1,6-dihydro-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



RN 812691-96-6 CAPLUS

CN	5-Pyrimidinecarbonitrile, 1,6-dihydro-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo-1-(3,4,5-trimethoxyphenyl)-	(CA INDEX NAME)
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L17 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 AN 2006:411890 CAPLUS
 DN 144:450725
 TI Preparation of pyrazolopyrimidinones and analogs, and their compositions
 as cannabinoid CB1 receptor inhibitors
 IN Liu, Hong; He, Xiaohui; Choi, Ha-Soon; Yang, Kunyong; Woodmansee, David;
 Wang, Zhicheng; Ellis, David Archer; Wu, Baogen; He, Yun; Nguyen, Truc
 Ngoc
 PA Irm LLC, Bermuda
 SO PCT Int. Appl., 259 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

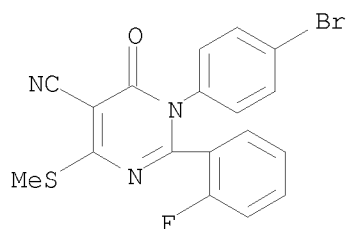
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2006047516	A2	20060504	WO 2005-US38361	20051026
	WO 2006047516	A3	20061012		
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	RW:		AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM		
	AU 2005299421	A1	20060504	AU 2005-299421	20051026
	CA 2581225	A1	20060504	CA 2005-2581225	20051026
	EP 1807429	A2	20070718	EP 2005-813001	20051026
	R:		AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR		
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	JP 2008518016	T	20080529	JP 2007-539039	20051026
	BR 2005017015	A	20080930	BR 2005-17015	20051026
	IN 2007DN02514	A	20070803	IN 2007-DN2514	20070403
	MX 200704936	A	20070625	MX 2007-4936	20070424
	KR 2007057980	A	20070607	KR 2007-709370	20070425
	NO 2007002352	A	20070531	NO 2007-2352	20070507
PRAI	US 2004-622508P	P	20041026		
	US 2005-672670P	P	20050418		
	WO 2005-US38361	W	20051026		

The instant application is entitled to the priority date of the provisional application filed 12/19/2003

OS CASREACT 144:450725; MARPAT 144:450725
 AB Title compds. I [Y = O, NH and derivs., S; R1 = (un)substituted Ph, heteroaryl, cycloalkyl, benzyl; R2 = (un)substituted Ph, OPh, heterocycloalkyl, heteroaryl; R3 = H, halo, OH, CN, etc.; R4 = (un)substituted hetero/aryl, alkyl, etc.; and their pharmaceutically acceptable salts, hydrates, solvates and isomers; with the exception of certain compds.] were prepared as selective cannabinoid CB1 receptor inhibitors. Thus, II was prepared, in 3 steps, starting from 5-amino-1-phenyl-1H-pyrazole-4-carboxylic acid Et ester and 2,4-dichlorobenzoyl chloride. Preferred compds. I showed a 100 fold selectivity for CB1 over CB2 receptor. Pharmaceutical compns. comprising I are useful for preventing and treating diseases or disorders associated

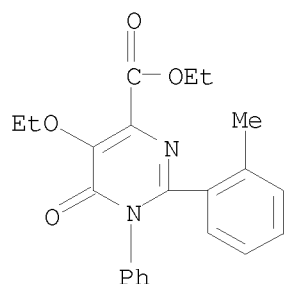
with the activity of CB1 receptor, e.g. metabolic disorders.

IT 885619-00-1P, 1-(4-Bromophenyl)-2-(2-fluorophenyl)-4-methylsulfanyl-6-oxo-1,6-dihydropyrimidine-5-carbonitrile
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate; preparation of pyrazolopyrimidinones and analogs as CB1 inhibitors)
 RN 885619-00-1 CAPLUS
 CN 5-Pyrimidinecarbonitrile, 1-(4-bromophenyl)-2-(2-fluorophenyl)-1,6-dihydro-4-(methylthio)-6-oxo- (CA INDEX NAME)

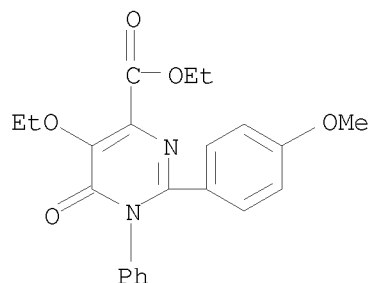


RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

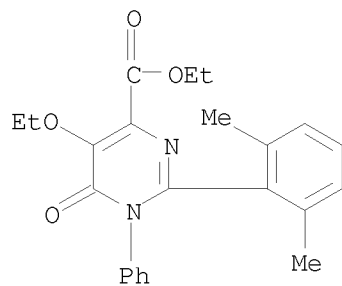
L17 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 AN 2006:406715 CAPLUS
 DN 144:468112
 TI Suzuki coupling at the 2-position of densely functionalized pyrimidones
 AU Colarusso, Stefania; Girardin, Melina; Conte, Immacolata; Narjes, Frank
 CS IRBM-Merc Research Laboratories Rome, Rome, 00040, Italy
 SO Synthesis (2006), (8), 1343-1350
 CODEN: SYNTBF; ISSN: 0039-7881
 PB Georg Thieme Verlag
 DT Journal
 LA English
 OS CASREACT 144:468112
 AB A variety of Et 1-substituted 2-aryl-5-ethoxy-6-oxo-1,6-dihydropyrimidine-4-carboxylates were synthesized by efficient thermal or microwave-promoted Suzuki coupling of 2-chloro-N1-substituted precursors.
 IT 886221-69-8P 886221-70-1P 886221-71-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of 2-aryldihydropyrimidinecarboxylates via palladium catalyzed thermal or microwave-promoted Suzuki coupling of chloro-substituted pyrimidinone intermediate with arylboronic acids)
 RN 886221-69-8 CAPLUS
 CN 4-Pyrimidinecarboxylic acid, 5-ethoxy-1,6-dihydro-2-(2-methylphenyl)-6-oxo-1-phenyl-, ethyl ester (CA INDEX NAME)



RN 886221-70-1 CAPLUS
 CN 4-Pyrimidinecarboxylic acid, 5-ethoxy-1,6-dihydro-2-(4-methoxyphenyl)-6-oxo-1-phenyl-, ethyl ester (CA INDEX NAME)



RN 886221-71-2 CAPLUS
 CN 4-Pyrimidinecarboxylic acid, 2-(2,6-dimethylphenyl)-5-ethoxy-1,6-dihydro-6-oxo-1-phenyl-, ethyl ester (CA INDEX NAME)



RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 AN 2005:1215763 CAPLUS
 DN 143:477975
 TI Preparation of pyrimidinones and quinazolinones as calcilytic compounds
 IN Luengo, Juan I.; Marquis, Robert W., Jr.; Xie, Ren; Yamashita, Dennis S.
 PA Smithkline Beecham Corporation, USA
 SO PCT Int. Appl., 34 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005108376	A1	20051117	WO 2005-US15224	20050503
	W:		AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW		
	RW:		BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG		
	EP 1742924	A1	20070117	EP 2005-744198	20050503
	R:		AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR, LV		
	JP 2007536239	T	20071213	JP 2007-511482	20050503
PRAI	US 2004-568585P	P	20040506		
	WO 2005-US15224	W	20050503		

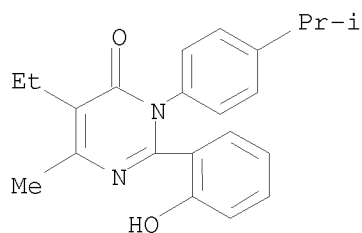
The instant application is eligible to the priority date of 12/19/03

OS CASREACT 143:477975; MARPAT 143:477975
 AB The title compds. I [R1, R2 = H, halo, CN, etc.; or R1 and R2 may be bonded together to form a carbocyclic, heterocyclic, aryl or heteroaryl ring; R3 = aryl or heteroaryl group which may have 1-5 substituents each selected from H, halo, CN, CF3, etc.; R4 = aryl which may have 1-3 substituents consisting of H, halo, CN, CF3, etc.; X = O or S], useful for treating a disease or disorder characterized by an abnormal bone or mineral homeostasis, were prepared E.g., a multi-step synthesis of 2-(2-hydroxyphenyl)-3-(4-isopropylphenyl)-5,6,7,8-tetrahydro-3H-quinazolin-4-one, starting from Et 2-aminocyclohex-1-enecarboxylate and 2-benzyloxybenzoyl chloride, was given. The methods for treating diseases or disorders such as osteosarcoma, periodontal disease, fracture healing, osteoarthritis, joint replacement, rheumatoid arthritis, Paget's disease, humoral hypercalcemia, malignancy and osteoporosis by administering the compound I alone or in combination with anti-resorptive agents are disclosed.
 IT 869564-58-9P 869564-60-3P 869564-62-5P
 869564-64-7P 869564-66-9P 869564-68-1P
 869564-70-5P 869564-72-7P 869564-74-9P
 869564-76-1P 869564-98-7P 869564-99-8P
 869565-00-4P 869565-01-5P 869565-02-6P
 869565-03-7P 869565-04-8P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrimidinones and quinazolinones as calcilytic compds.)

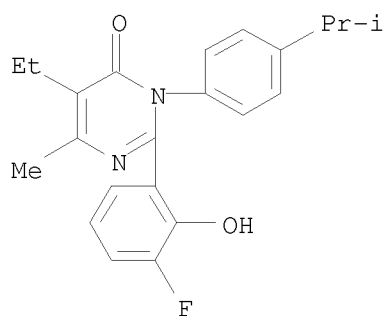
RN 869564-58-9 CAPLUS

CN 4(3H)-Pyrimidinone, 5-ethyl-2-(2-hydroxyphenyl)-6-methyl-3-[4-(1-methylethyl)phenyl]- (CA INDEX NAME)



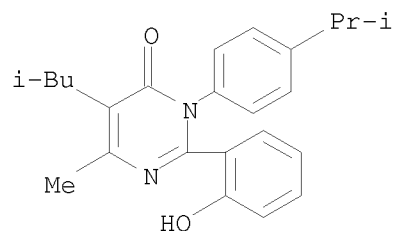
RN 869564-60-3 CAPLUS

CN 4(3H)-Pyrimidinone, 5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-[4-(1-methylethyl)phenyl]- (CA INDEX NAME)



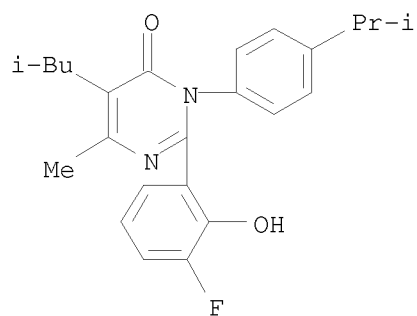
RN 869564-62-5 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-3-[4-(1-methylethyl)phenyl]-5-(2-methylpropyl)- (CA INDEX NAME)



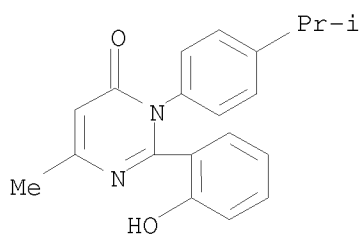
RN 869564-64-7 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-[4-(1-methylethyl)phenyl]-5-(2-methylpropyl)- (CA INDEX NAME)



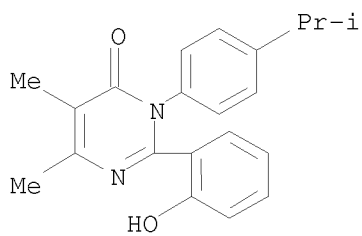
RN 869564-66-9 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-3-[4-(1-methylethyl)phenyl]- (CA INDEX NAME)



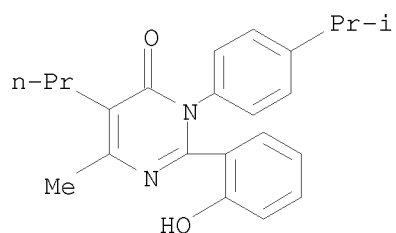
RN 869564-68-1 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-5,6-dimethyl-3-[4-(1-methylethyl)phenyl]- (CA INDEX NAME)



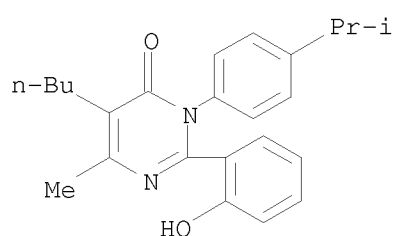
RN 869564-70-5 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-3-[4-(1-methylethyl)phenyl]-5-propyl- (CA INDEX NAME)



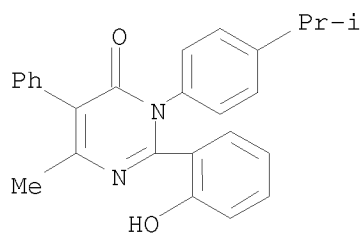
RN 869564-72-7 CAPLUS

CN 4(3H)-Pyrimidinone, 5-butyl-2-(2-hydroxyphenyl)-6-methyl-3-[4-(1-methylethyl)phenyl]- (CA INDEX NAME)



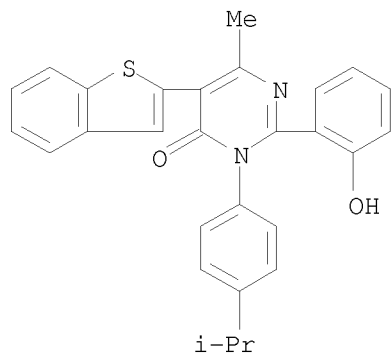
RN 869564-74-9 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-3-[4-(1-methylethyl)phenyl]-5-phenyl- (CA INDEX NAME)



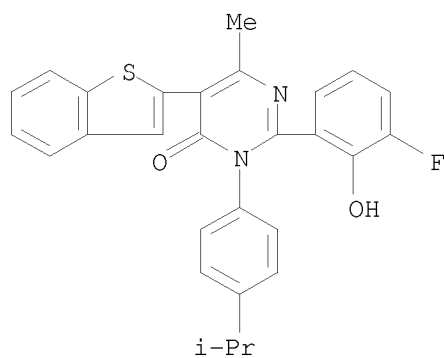
RN 869564-76-1 CAPLUS

CN 4(3H)-Pyrimidinone, 5-benzo[b]thien-2-yl-2-(2-hydroxyphenyl)-6-methyl-3-[4-(1-methylethyl)phenyl]- (CA INDEX NAME)



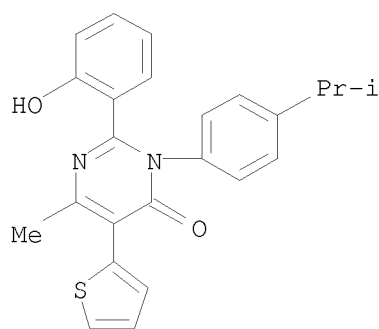
RN 869564-98-7 CAPLUS

CN 4(3H)-Pyrimidinone, 5-benzo[b]thien-2-yl-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-[4-(1-methylethyl)phenyl]- (CA INDEX NAME)



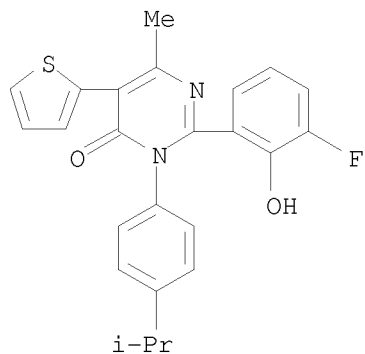
RN 869564-99-8 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-3-[4-(1-methylethyl)phenyl]-5-(2-thienyl)- (CA INDEX NAME)



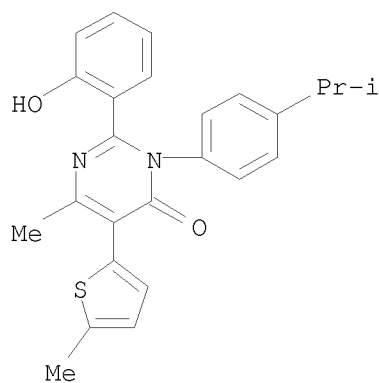
RN 869565-00-4 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-[4-(1-methylethyl)phenyl]-5-(2-thienyl)- (CA INDEX NAME)



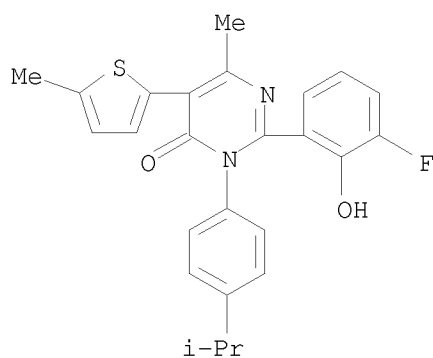
RN 869565-01-5 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-3-[4-(1-methylethyl)phenyl]-5-(5-methyl-2-thienyl)- (CA INDEX NAME)



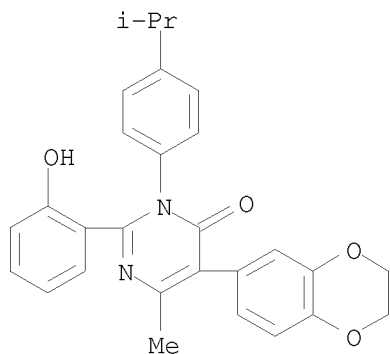
RN 869565-02-6 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-[4-(1-methylethyl)phenyl]-5-(5-methyl-2-thienyl)- (CA INDEX NAME)



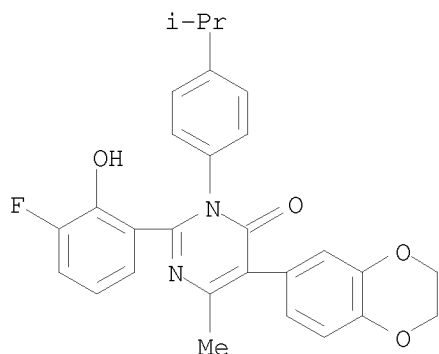
RN 869565-03-7 CAPLUS

CN 4(3H)-Pyrimidinone, 5-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-(2-hydroxyphenyl)-6-methyl-3-[4-(1-methylethyl)phenyl]- (CA INDEX NAME)



RN 869565-04-8 CAPLUS

CN 4(3H)-Pyrimidinone, 5-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-[4-(1-methylethyl)phenyl]- (CA INDEX NAME)



IT 869564-88-5P 869564-94-3P 869564-95-4P

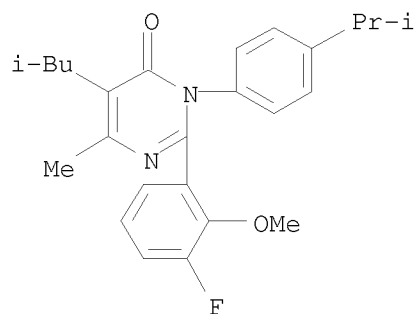
869564-96-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

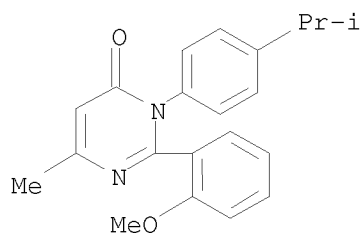
(preparation of pyrimidinones and quinazolinones as calcilytic compds.)

RN 869564-88-5 CAPLUS

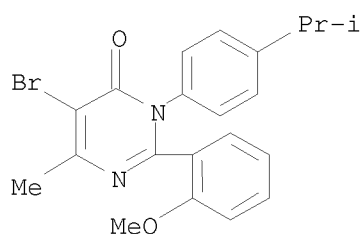
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-methoxyphenyl)-6-methyl-3-[4-(1-methylethyl)phenyl]-5-(2-methylpropyl)- (CA INDEX NAME)



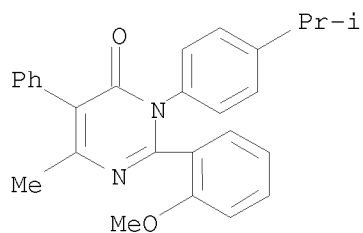
RN 869564-94-3 CAPLUS
 CN 4(3H)-Pyrimidinone, 2-(2-methoxyphenyl)-6-methyl-3-[4-(1-methylethyl)phenyl]- (CA INDEX NAME)



RN 869564-95-4 CAPLUS
 CN 4(3H)-Pyrimidinone, 5-bromo-2-(2-methoxyphenyl)-6-methyl-3-[4-(1-methylethyl)phenyl]- (CA INDEX NAME)



RN 869564-96-5 CAPLUS
 CN 4(3H)-Pyrimidinone, 2-(2-methoxyphenyl)-6-methyl-3-[4-(1-methylethyl)phenyl]-5-phenyl- (CA INDEX NAME)



RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

AN 2005:1075505 CAPLUS

DN 143:367312

TI Preparation of novel condensed pyrimidones as cyclooxygenase inhibitors

IN Agarwal, Shiv Kumar; Tadiparthi, Ravi Kumar; Aggarwal, Pawan; Shivkumar, Savithri

PA Orchid Chemicals & Pharmaceuticals Ltd., India

SO PCT Int. Appl., 38 pp.

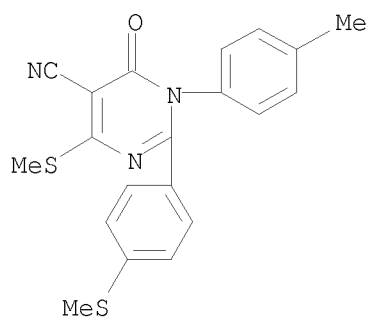
CODEN: PIXXD2

DT Patent

LA English

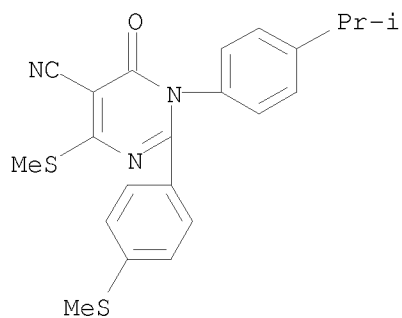
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005091711	A2	20051006	WO 2005-IB736	20050322
	WO 2005091711	A3	20060309		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
	RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	IN 2004CH00270	A	20051202	IN 2004-CH270	20040324
PRAI	IN 2004-CH270	A	20040324		
OS	CASREACT 143:367312; MARPAT 143:367312				
AB	The title compds. I [X = O, S; Ar1, Ar2 = (un)substituted aryl, heteroaryl, heterocyclyl; R1, R2 = H, OH, NO2, etc.], useful for lowering plasma concns. of cytokines, and for decreasing cyclooxygenase activity, were prepared Thus, reacting guanidine.HCl with 5-cyano-1-(4-methylphenyl)-4-methylthio-2-(4-methylthiophenyl)-1,6-dihydropyrimidin-6-one in the presence of anhydrous K2CO3 in DMF afforded 23% I [X = O; Ar1 = 4-MeC6H4; Ar2 = 4-(MeS)C6H4; R1, R2 = NH2] which showed 29% COX-2 inhibition and 53% IL-6 inhibition. The present invention relates also to the pharmaceutically acceptable salts and pharmaceutically acceptable compns. containing compds. I.				
IT	613663-83-5, 5-Cyano-1-(4-methylphenyl)-4-methylthio-2-(4-methylthiophenyl)-1,6-dihydropyrimidin-6-one 812691-92-2, 5-Cyano-1-(4-isopropylphenyl)-4-methylthio-2-(4-methylthiophenyl)-1,6-dihydropyrimidin-6-one 812691-93-3, 5-Cyano-1-(3,4-dimethylphenyl)-4-methylthio-2-(4-methylthiophenyl)-1,6-dihydropyrimidin-6-one				
	RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of novel condensed pyrimidones as cyclooxygenase inhibitors)				
RN	613663-83-5 CAPLUS				
CN	5-Pyrimidinecarbonitrile, 1,6-dihydro-1-(4-methylphenyl)-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)				



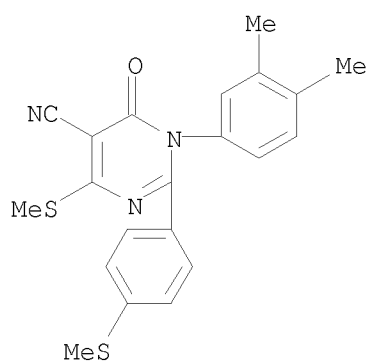
RN 812691-92-2 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1,6-dihydro-1-[4-(1-methylethyl)phenyl]-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



RN 812691-93-3 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1-(3,4-dimethylphenyl)-1,6-dihydro-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 AN 2005:588550 CAPLUS
 DN 143:115555
 TI Preparation of 2-phenylpyrimidinone mitotic kinesin inhibitors
 IN Arrington, Kenneth L.; Fraley, Mark E.; Hartman, George D.
 PA Merck & Co., Inc., USA
 SO PCT Int. Appl., 52 pp.
 CODEN: PIXXD2

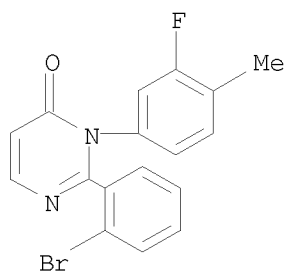
DT Patent
 LA English

Applicant's

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005060654	A2	20050707	WO 2004-US42171	20041215
	WO 2005060654	A3	20051208		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, SM			
	RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	AU 2004305069	A1	20050707	AU 2004-305069	20041215
	CA 2547209	A1	20050707	CA 2004-2547209	20041215
	EP 1697331	A2	20060906	EP 2004-814365	20041215
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS			
	CN 1898215	A	20070117	CN 2004-80038124	20041215
	JP 2007518711	T	20070712	JP 2006-545404	20041215
	IN 2006DN02999	A	20070803	IN 2006-DN2999	20060525
	US 20070129356	A1	20070607	US 2006-582826	20060614
PRAI	US 2003-531554P	P	20031219		
	WO 2004-US42171	W	20041215		
OS	CASREACT 143:115555; MARPAT 143:115555				
AB	Title compds. I [R1 = H, alkyl, aryl, alkenyl, etc.; R2 = acyl, carboxy, etc.; R3a-3b = H, acyl, alkyl, etc.; p = 1-3] are prepared For instance, 2-(2-bromophenyl)-3-(3-fluoro-4-methylphenyl)pyrimidin-4(3H)-one (II) is prepared in 3 steps from 2-bromobenzonitrile, 3-fluoro-4-methylaniline, DMF di-Me acetal and trimethylsilylketene. II exhibits IC50 ≤ 50 μM for KSP kinesin. I are useful for the treatment of cancer.				
IT	857086-87-4P, 2-(2-Bromophenyl)-3-(3-fluoro-4-methylphenyl)pyrimidin-4(3H)-one				
	RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)				
	(preparation of 2-phenylpyrimidinone mitotic kinesin inhibitors)				
RN	857086-87-4 CAPLUS				
CN	4(3H)-Pyrimidinone, 2-(2-bromophenyl)-3-(3-fluoro-4-methylphenyl)- (CA INDEX NAME)				

10/582,826



RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

AN 2004:1127094 CAPLUS

DN 142:74592

TI Preparation of novel pyrimidones for treating inflammation and immunol. diseases

IN Agarwal, Shiv Kumar; Tadiparthi, Ravikumar; Aggarwal, Pawan; Shivakumar, Savithiri; Dey, Debendranath; Nag, Biswajit

PA Orchid Chemical & Pharmaceuticals Limited, India

SO U.S. Pat. Appl. Publ., 42 pp., Cont.-in-part of U.S. Ser. No. 409,045. CODEN: USXXCO

DT Patent

LA English

FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 20040259891	A1	20041223	US 2004-827368	20040420
	US 7365069	B2	20080429		
	IN 2002MA00266	A	20050304	IN 2002-MA266	20020410
	US 20030225075	A1	20031204	US 2003-409045	20030409
	US 20060194799	A1	20060831	US 2006-414229	20060501
	US 7399760	B2	20080715		
PRAI	IN 2002-MA266	A	20020410		
	US 2003-409045	A2	20030409		
	US 2003-409153	A3	20030409		

OS MARPAT 142:74592

AB The title compds. [I; X = O, S, NR (R = H, OH, acyl, etc.); A, B = (hetero)aryl; R1, R3 = H, SR7, SOpR8 (R7 = H, alkyl, aryl; R8 = halo, alkyl, NH2, acylamino, arylamino, aryl; p = 1-2); R2, R4 = H, halo, OH, etc.; R5, R6 = H, halo, OH, NO2, etc.; n, m = 0-4], useful for treating inflammation and immunol. diseases mediated by cytokines such as TNF- α , IL-1, IL-6, IL-1 β , IL-8 and cyclooxygenase such as COX-2 and COX-3, were prepared Thus, reacting Et 2-cyano-3,3-dimethylthioacrylate with N-(4-methylthiophenyl)-4-fluorobenzamidine (preparation given) afforded II which showed 53.38% COX-2 inhibition. The pharmaceutical compns. comprising the compound I are disclosed.

IT 613663-79-9P 613663-83-5P 812691-93-3P

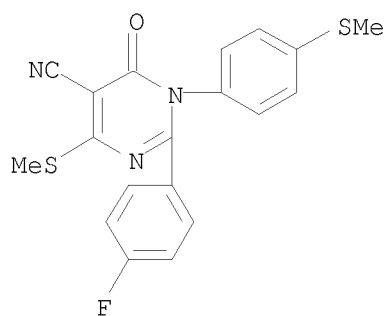
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RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of novel pyrimidones for treating inflammation and immunol. diseases)

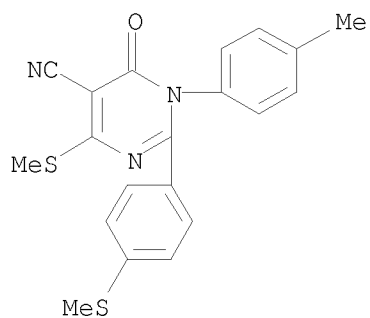
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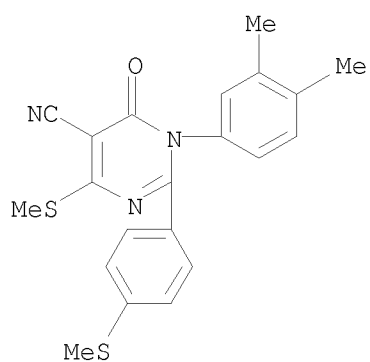
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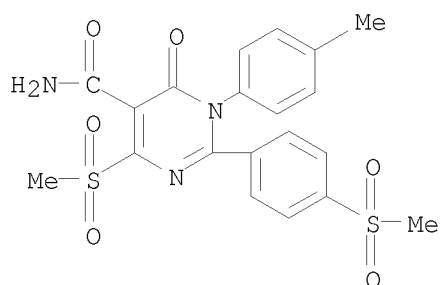
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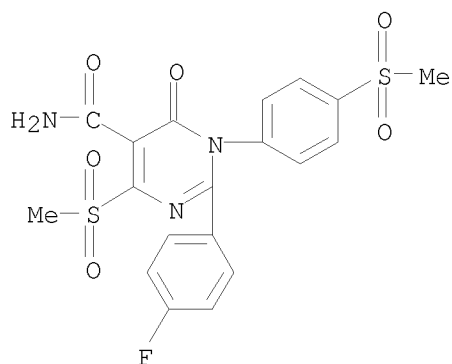
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CN 5-Pyrimidinecarboxamide, 1,6-dihydro-1-(4-methylphenyl)-4-(methylsulfonyl)-2-[4-(methylsulfonyl)phenyl]-6-oxo- (CA INDEX NAME)



RN 812692-31-2 CAPLUS

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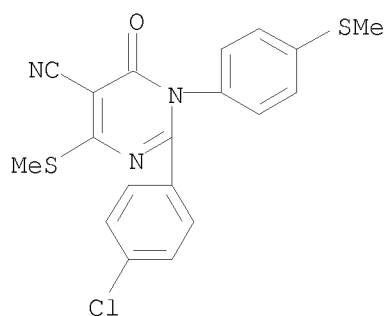
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 812692-74-3P 812692-75-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of novel pyrimidones for treating inflammation and immunol. diseases)

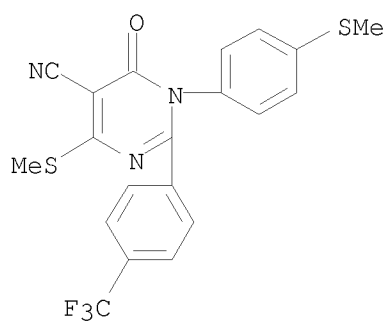
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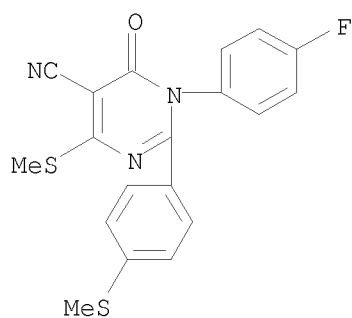
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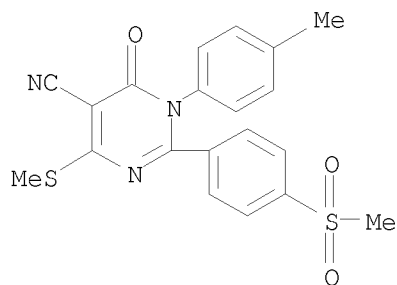
RN 613663-82-4 CAPLUS

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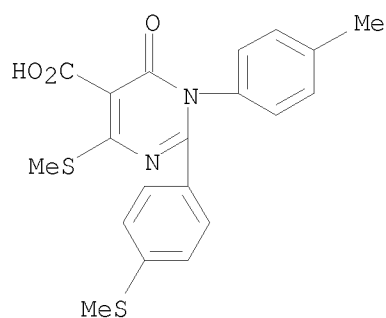
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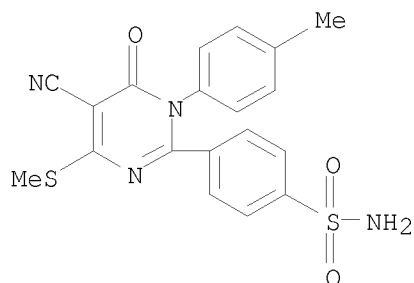
RN 613663-85-7 CAPLUS

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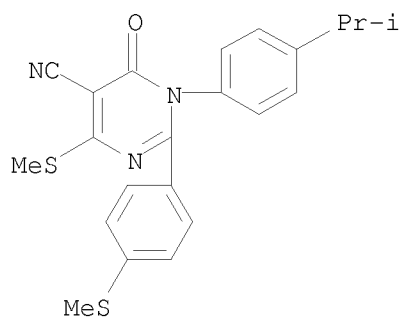
RN 613663-95-9 CAPLUS

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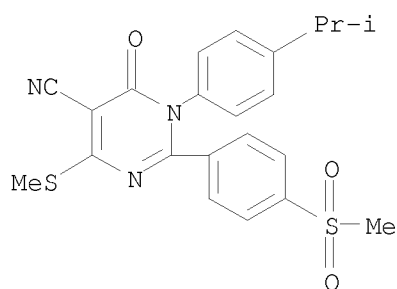
RN 812691-92-2 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1,6-dihydro-1-[4-(1-methylethyl)phenyl]-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



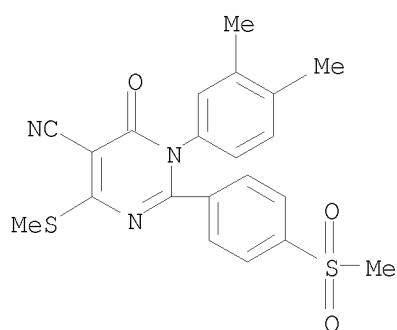
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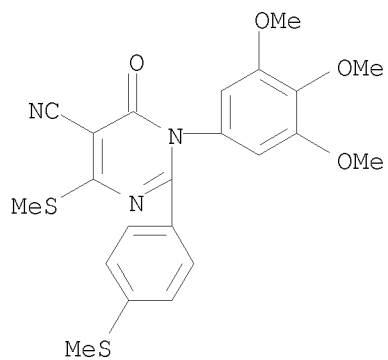
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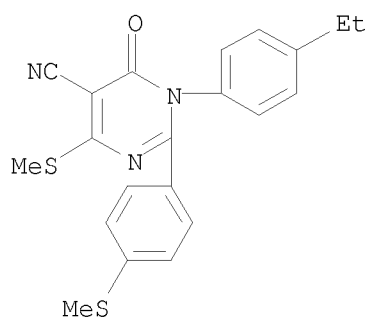
RN 812691-96-6 CAPLUS

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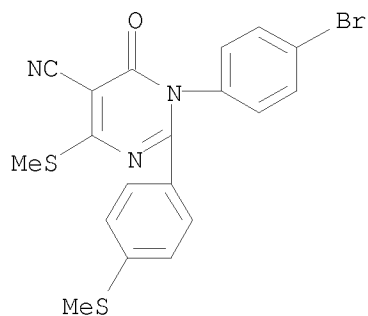
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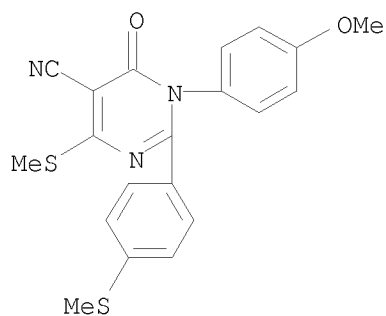
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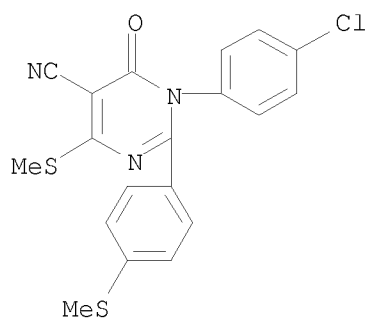
RN 812691-99-9 CAPLUS

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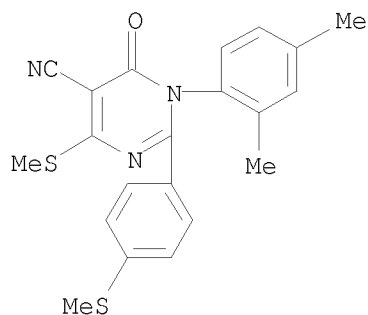
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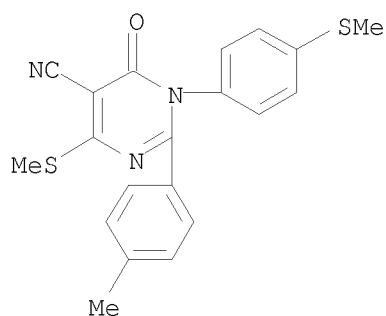
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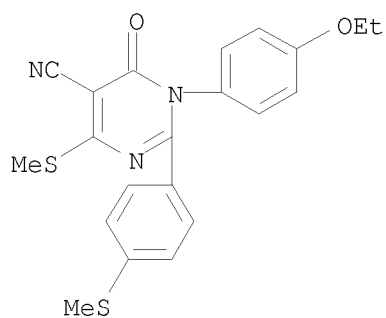
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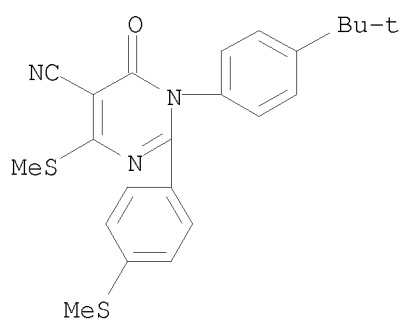
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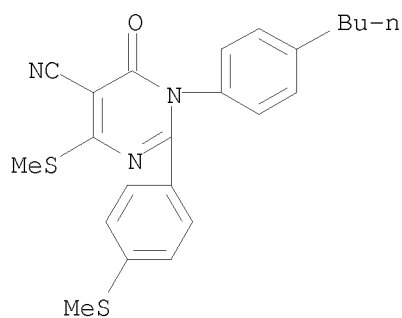
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CN 5-Pyrimidinecarbonitrile, 1-[4-(1,1-dimethylethyl)phenyl]-1,6-dihydro-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



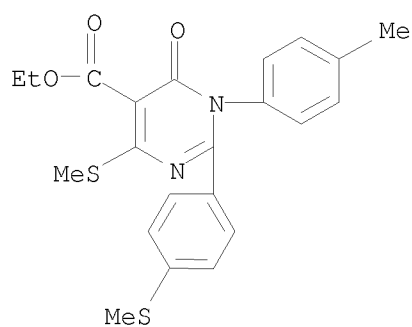
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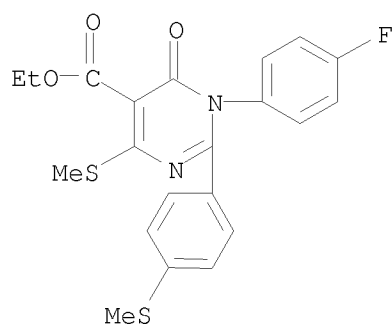
RN 812692-24-3 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,6-dihydro-1-(4-methylphenyl)-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo-, ethyl ester (CA INDEX NAME)



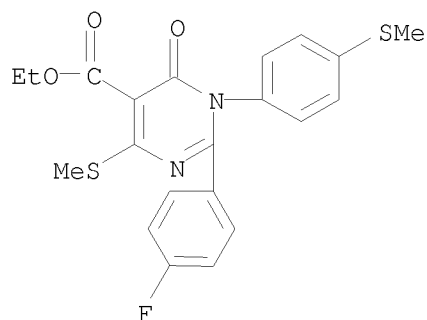
RN 812692-25-4 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 1-(4-fluorophenyl)-1,6-dihydro-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo-, ethyl ester (CA INDEX NAME)



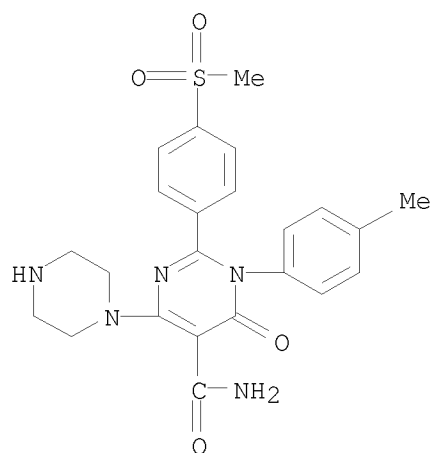
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CN 5-Pyrimidinecarboxylic acid, 2-(4-fluorophenyl)-1,6-dihydro-4-(methylthio)-1-[4-(methylthio)phenyl]-6-oxo-, ethyl ester (CA INDEX NAME)



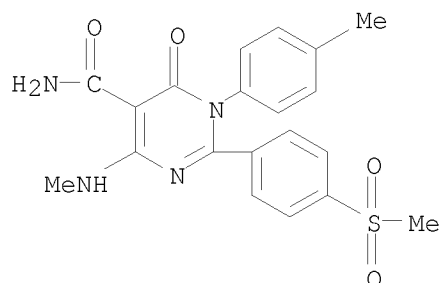
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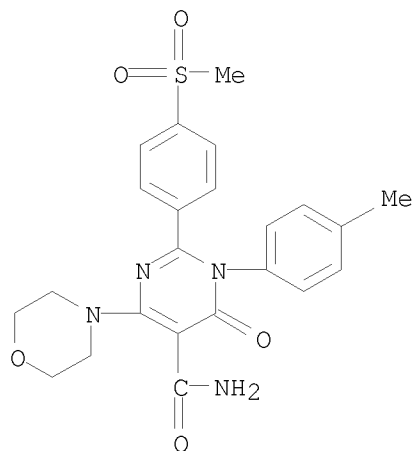
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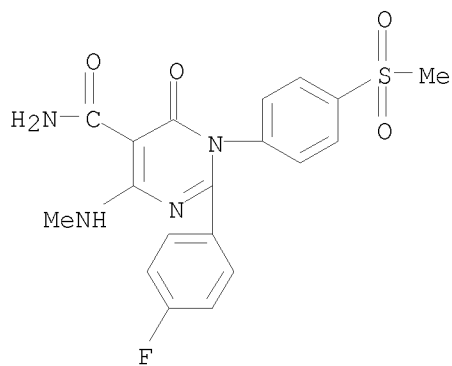
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CN 5-Pyrimidinecarboxamide, 1,6-dihydro-1-(4-methylphenyl)-2-[4-(methylsulfonyl)phenyl]-4-(4-morpholinyl)-6-oxo- (CA INDEX NAME)



RN 812692-32-3 CAPLUS

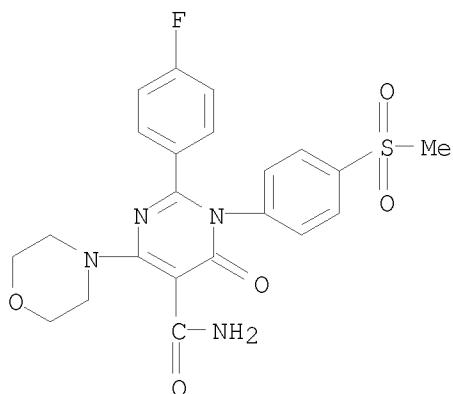
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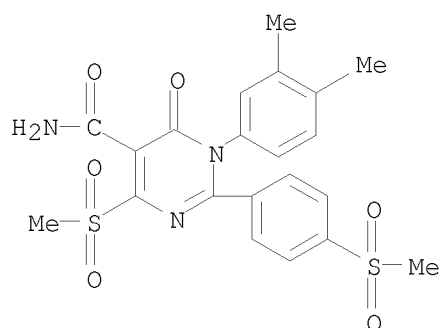
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10/582,826



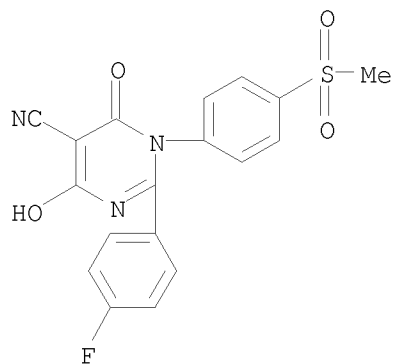
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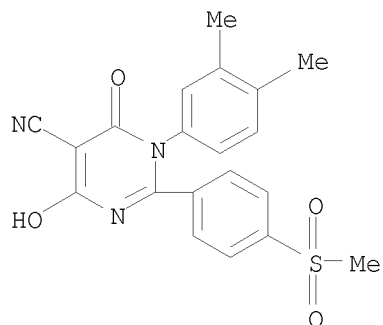
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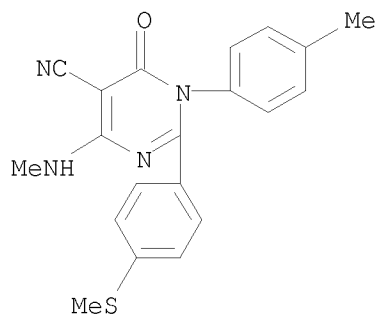
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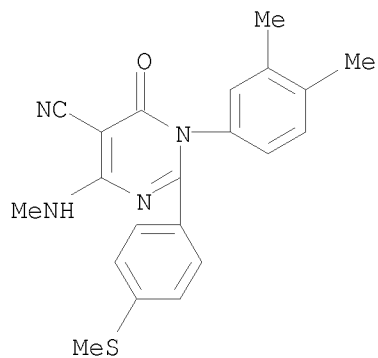
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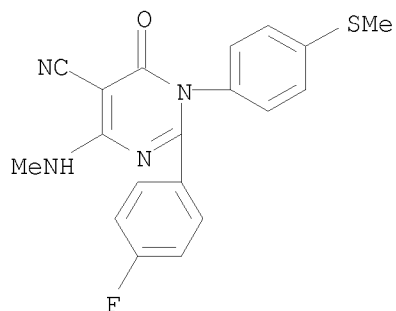
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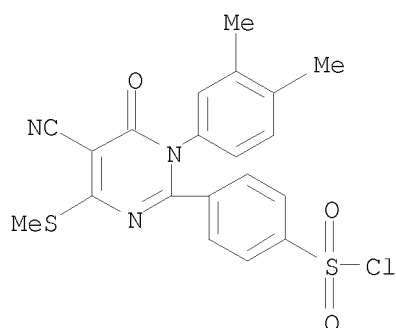
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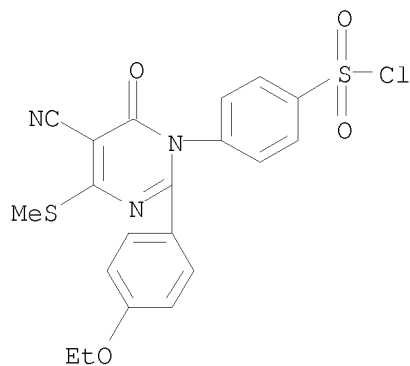
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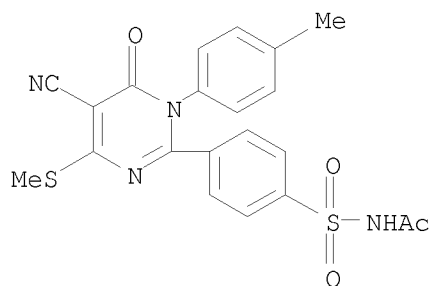
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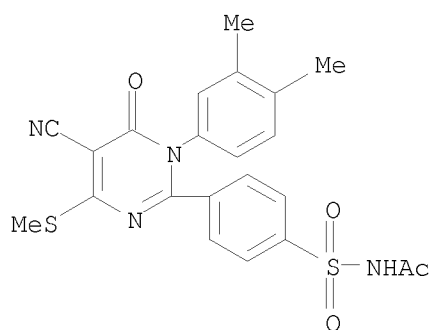
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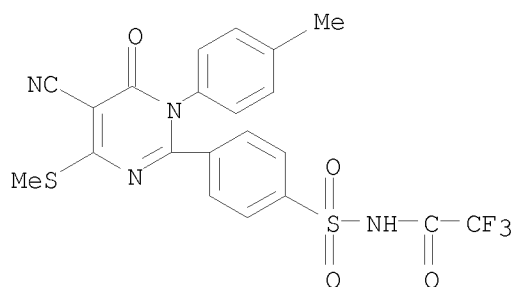
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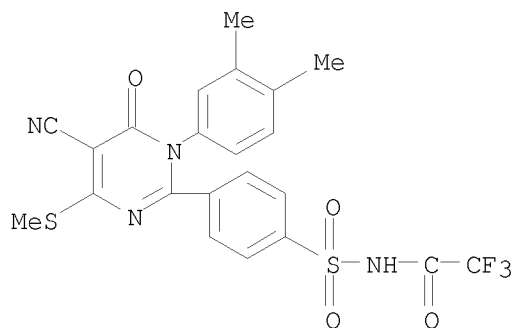
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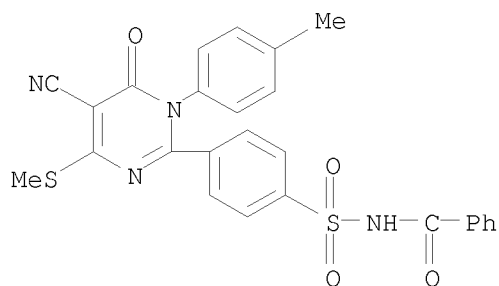
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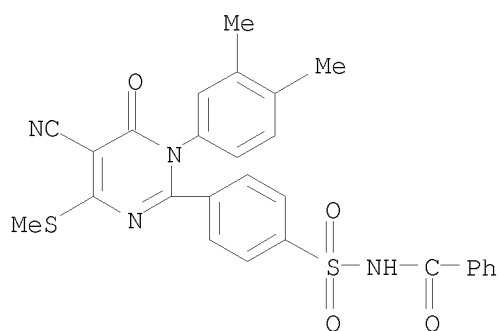
RN 812692-74-3 CAPLUS

CN Benzamide, N-[[4-[5-cyano-1,6-dihydro-1-(4-methylphenyl)-4-(methylthio)-6-oxo-2-pyrimidinyl]phenyl]sulfonyl]- (CA INDEX NAME)



RN 812692-75-4 CAPLUS

CN Benzamide, N-[[4-[5-cyano-1-(3,4-dimethylphenyl)-1,6-dihydro-4-(methylthio)-6-oxo-2-pyrimidinyl]phenyl]sulfonyl]- (CA INDEX NAME)



IT 812692-69-6

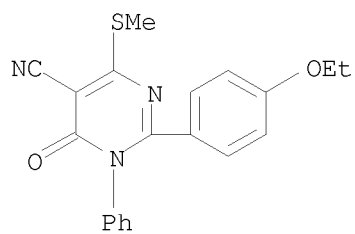
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of novel pyrimidones for treating inflammation and immunol. diseases)

RN 812692-69-6 CAPLUS

CN 5-Pyrimidinecarbonitrile, 2-(4-ethoxyphenyl)-1,6-dihydro-4-(methylthio)-6-

10/582,826

oxo-1-phenyl- (CA INDEX NAME)



RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 AN 2003:818406 CAPLUS
 DN 139:323531
 TI Preparation of novel pyrimidones for treating inflammation and immunol. diseases
 IN Agarwal, Shiv Kumar; Tadiparthi, Ravikumar; Aggarwal, Pawan; Shivakumar, Savithiri; Dey, Debendranath; Nag, Biswajit
 PA Orchid Chemicals & Pharmaceuticals Limited, India
 SO PCT Int. Appl., 47 pp.
 CODEN: PIXXD2
 DT Patent
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	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003084938	A2	20031016	WO 2003-IB1306	20030410
	WO 2003084938	A3	20040205		
	W:				
	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW:				
	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
IN	2002MA00266	A	20050304	IN 2002-MA266	20020410
US	20030232813	A1	20031218	US 2003-409161	20030409
US	20040009975	A1	20040115	US 2003-409153	20030409
US	7101873	B2	20060905		
CA	2481825	A1	20031016	CA 2003-2481825	20030410
AU	2003216592	A1	20031020	AU 2003-216592	20030410
EP	1492774	A2	20050105	EP 2003-712500	20030410
	R:				
	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN	1656080	A	20050817	CN 2003-812546	20030410
JP	2005535570	T	20051124	JP 2003-582135	20030410
IN	2004CH00353	A	20060526	IN 2004-CH353	20040419
US	20060194799	A1	20060831	US 2006-414229	20060501
US	7399760	B2	20080715		
IN	2006CH02100	A	20081128	IN 2006-CH2100	20061113
IN	2006CH02101	A	20081128	IN 2006-CH2101	20061113
PRAI	IN 2002-MA266	A	20020410		
	US 2003-409153	A3	20030409		
	WO 2003-IB1306	W	20030410		
OS	MARPAT 139:323531				
AB	Th title compds. [I; X = O, S, NR (R = H, OH, acyl, etc.); A, B = (hetero)aryl; R1, R3 = SR7, SOpR8 (R7 = alkyl, aryl; R8 = alkyl, NH2, aryl; p = 1-2); R2, R4 = H, halo, OH, etc.; R5, R6 = H, halo, OH, NO2, etc.; n, m = 0-2], useful for treating inflammation and immunol. diseases mediated by cytokines such as TNF- α , IL-1, IL-6, IL-1 β , IL-8 and cyclooxygenase such as COX-2 and COX-3, were prepared and formulated. Thus, reacting Et 2-cyano-3,3-dimethylthioacrylate with N-(4-methylthiophenyl)-4-fluorobenzamidine (preparation given) afforded II which showed 53.38% COX-2 inhibition. Pharmaceutical composition comprising the compound I is claimed.				

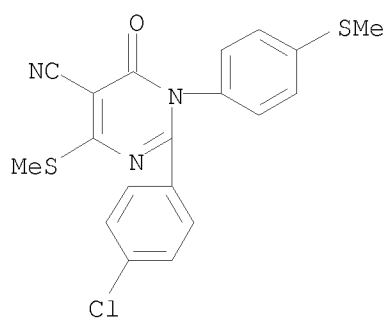
IT 613663-78-8P 613663-79-9P 613663-81-3P
 613663-82-4P 613663-83-5P 613663-84-6P
 613663-85-7P 613663-92-6P 613663-93-7P
 613663-94-8P 613663-95-9P 613663-96-0P
 613663-97-1P 613663-98-2P 613664-00-9P
 613664-01-0P 613664-02-1P 613664-03-2P
 613664-04-3P 613664-05-4P 613664-07-6P
 613664-09-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(preparation of novel pyrimidones for treating inflammation and immunol.
 diseases)

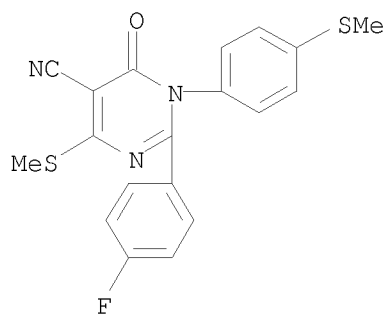
RN 613663-78-8 CAPLUS

CN 5-Pyrimidinecarbonitrile, 2-(4-chlorophenyl)-1,6-dihydro-4-(methylthio)-1-
 [4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



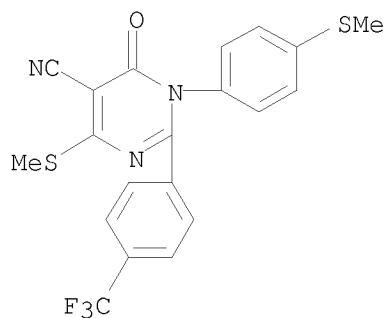
RN 613663-79-9 CAPLUS

CN 5-Pyrimidinecarbonitrile, 2-(4-fluorophenyl)-1,6-dihydro-4-(methylthio)-1-
 [4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



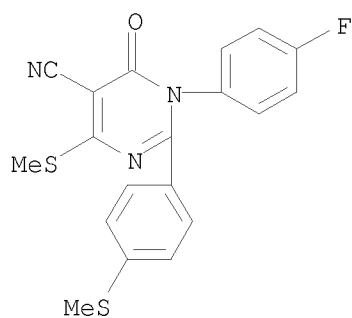
RN 613663-81-3 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1,6-dihydro-4-(methylthio)-1-[4-
 (methylthio)phenyl]-6-oxo-2-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



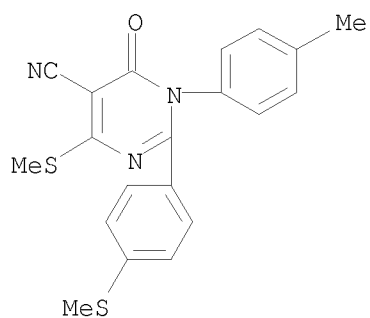
RN 613663-82-4 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1-(4-fluorophenyl)-1,6-dihydro-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



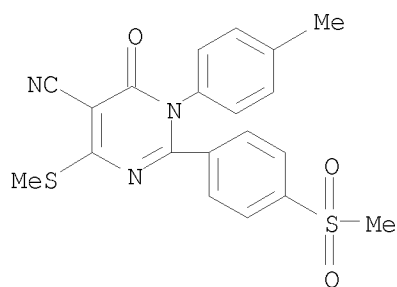
RN 613663-83-5 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1,6-dihydro-1-(4-methylphenyl)-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



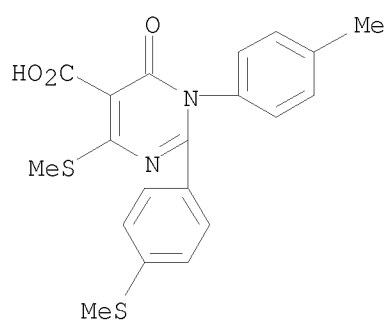
RN 613663-84-6 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1,6-dihydro-1-(4-methylphenyl)-2-[4-(methylsulfonyl)phenyl]-4-(methylthio)-6-oxo- (CA INDEX NAME)



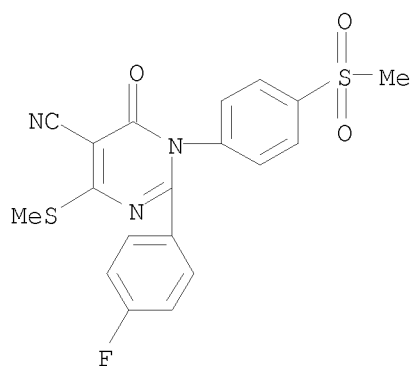
RN 613663-85-7 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,6-dihydro-1-(4-methylphenyl)-4-(methylthio)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



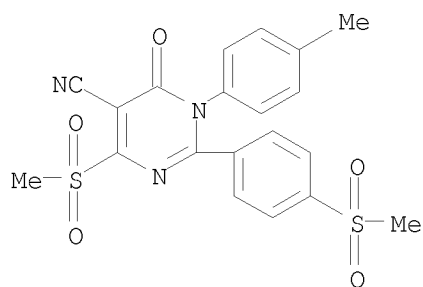
RN 613663-92-6 CAPLUS

CN 5-Pyrimidinecarbonitrile, 2-(4-fluorophenyl)-1,6-dihydro-1-[4-(methylsulfonyl)phenyl]-4-(methylthio)-6-oxo- (CA INDEX NAME)



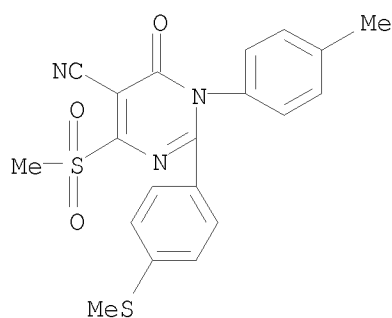
RN 613663-93-7 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1,6-dihydro-1-(4-methylphenyl)-4-(methylsulfonyl)-2-[4-(methylsulfonyl)phenyl]-6-oxo- (CA INDEX NAME)



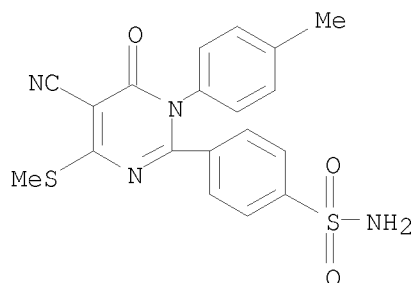
RN 613663-94-8 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1,6-dihydro-1-(4-methylphenyl)-4-(methylsulfonyl)-2-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



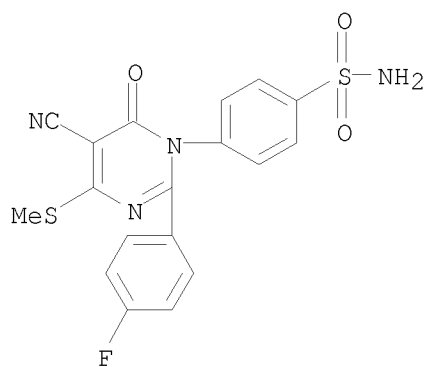
RN 613663-95-9 CAPLUS

CN Benzenesulfonamide, 4-[5-cyano-1,6-dihydro-1-(4-methylphenyl)-4-(methylthio)-6-oxo-2-pyrimidinyl]- (CA INDEX NAME)



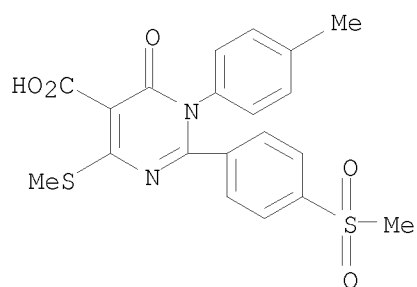
RN 613663-96-0 CAPLUS

CN Benzenesulfonamide, 4-[5-cyano-2-(4-fluorophenyl)-4-(methylthio)-6-oxo-1(6H)-pyrimidinyl]- (CA INDEX NAME)



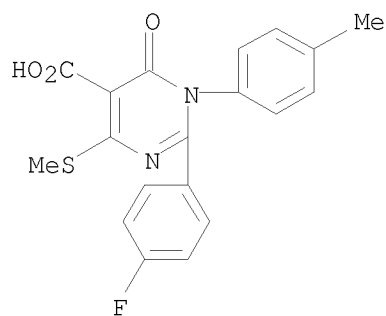
RN 613663-97-1 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,6-dihydro-1-(4-methylphenyl)-2-[4-(methylsulfonyl)phenyl]-4-(methylthio)-6-oxo- (CA INDEX NAME)



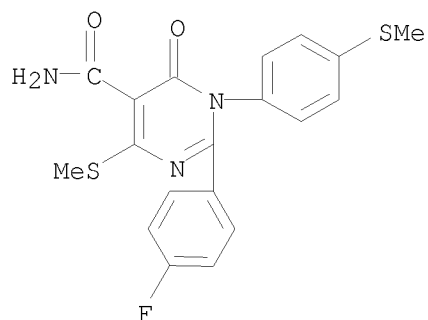
RN 613663-98-2 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 2-(4-fluorophenyl)-1,6-dihydro-1-(4-methylphenyl)-4-(methylthio)-6-oxo- (CA INDEX NAME)



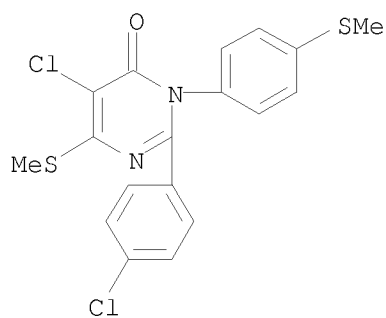
RN 613664-00-9 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-(4-fluorophenyl)-1,6-dihydro-4-(methylthio)-1-[4-(methylthio)phenyl]-6-oxo- (CA INDEX NAME)



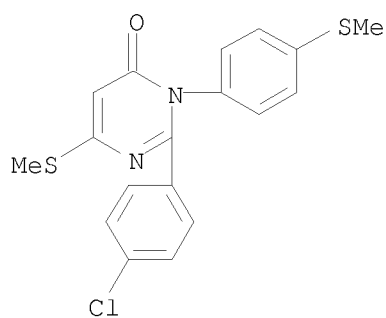
RN 613664-01-0 CAPLUS

CN 4(3H)-Pyrimidinone, 5-chloro-2-(4-chlorophenyl)-6-(methylthio)-3-[4-(methylthio)phenyl]- (CA INDEX NAME)



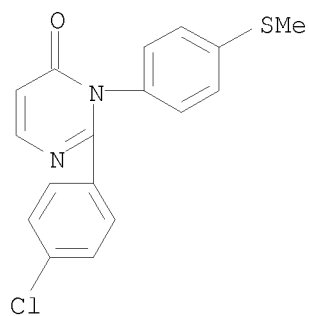
RN 613664-02-1 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(4-chlorophenyl)-6-(methylthio)-3-[4-(methylthio)phenyl]- (CA INDEX NAME)



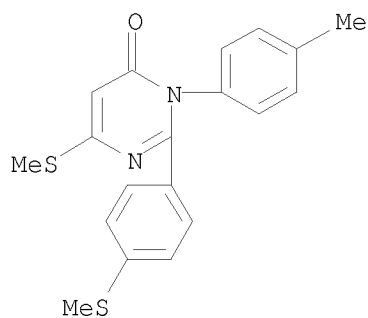
RN 613664-03-2 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(4-chlorophenyl)-3-[4-(methylthio)phenyl]- (CA INDEX NAME)



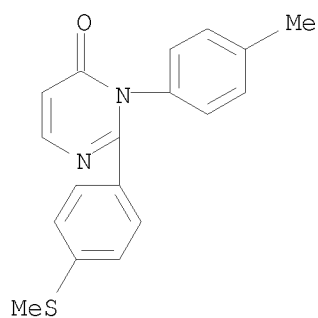
RN 613664-04-3 CAPLUS

CN 4(3H)-Pyrimidinone, 3-(4-methylphenyl)-6-(methylthio)-2-[4-(methylthio)phenyl]- (CA INDEX NAME)



RN 613664-05-4 CAPLUS

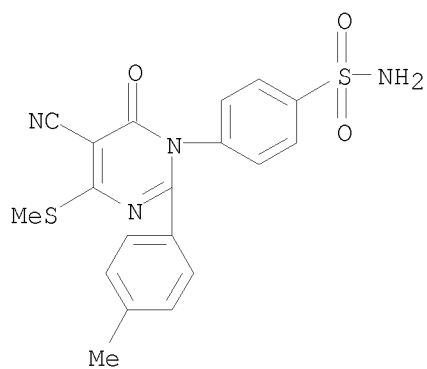
CN 4(3H)-Pyrimidinone, 3-(4-methylthiophenyl)-2-[4-(methylthio)phenyl]- (CA INDEX NAME)



RN 613664-07-6 CAPLUS

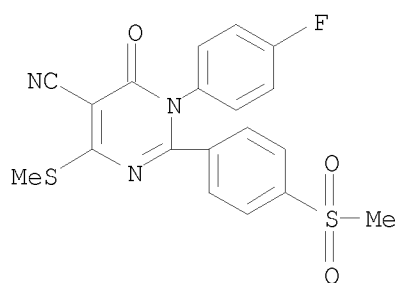
CN Benzenesulfonamide, 4-[5-cyano-2-(4-methylthiophenyl)-4-(methylthio)-6-oxo-1(6H)-pyrimidinyl]- (CA INDEX NAME)

10/582,826



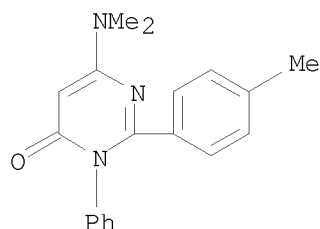
RN 613664-09-8 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1-(4-fluorophenyl)-1,6-dihydro-2-[4-(methylsulfonyl)phenyl]-4-(methylthio)-6-oxo- (CA INDEX NAME)

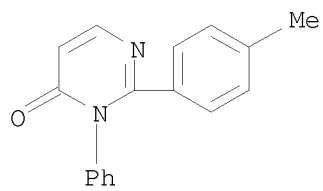


RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 AN 2002:33216 CAPLUS
 DN 136:340653
 TI A facile synthesis of 4(3H)-pyrimidinones via [4+2] cycloaddition
 utilizing (trimethylsilyl)ketene
 AU Arai, Shigeru; Sakurai, Takuya; Asakura, Hitomi; Fuma, Shin-Ya; Shioiri,
 Takayuki; Aoyama, Toyohiko
 CS Graduate School of Pharmaceutical Sciences, Nagoya City University,
 Nagoya, 467-8603, Japan
 SO Heterocycles (2001), 55(12), 2283-2287
 CODEN: HTCYAM; ISSN: 0385-5414
 PB Japan Institute of Heterocyclic Chemistry
 DT Journal
 LA English
 OS CASREACT 136:340653
 AB The [4+2]cycloaddn. reaction utilizing (trimethylsilyl)ketene with
 1,3-diaza-1,3-dienes smoothly proceeded to give the desired cycloadducts,
 4(3H)-pyrimidinones, in moderate to high yields. The 1,3-diaza-1,3-dienes
 included N-[(dimethylamino)methylene]-N'-phenylbenzenecarboximidamide,
 N-[(dimethylamino)methylene]-N'-(4-methylphenyl)benzenecarboximidamide,
 N-[(dimethylamino)methylene]-4-methyl-N'-phenylbenzenecarboximidamide,
 N-[(dimethylamino)methylene]-N'-phenyl-2-naphthalenecarboximidamide,
 [(dimethylamino)methylene]phenylcarbamidodithioic acid Me ester, and
 similar compds. For example, the cycloaddn. of (trimethylsilyl)ketene
 with N-[(dimethylamino)methylene]-N'-phenylbenzenecarboximidamide gave
 2,3-diphenyl-4(3H)-pyrimidinone (I) in 94% yield in Et acetate. When the
 reaction was run in toluene as solvent the yield of I was 60% and
 6-(dimethylamino)-2,3-diphenyl-4(3H)-pyrimidinone (21%) was obtained as
 byproduct.
 IT 417755-31-8P
 RL: BYP (Byproduct); PREP (Preparation)
 (preparation of 4(3H)-pyrimidinones via [4+2] cycloaddn. of
 (trimethylsilyl)ketene with 1,3-diaza-1,3-dienes)
 RN 417755-31-8 CAPLUS
 CN 4(3H)-Pyrimidinone, 6-(dimethylamino)-2-(4-methylphenyl)-3-phenyl- (CA
 INDEX NAME)



IT 417754-93-9P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of 4(3H)-pyrimidinones via [4+2] cycloaddn. of
 (trimethylsilyl)ketene with 1,3-diaza-1,3-dienes)
 RN 417754-93-9 CAPLUS
 CN 4(3H)-Pyrimidinone, 2-(4-methylphenyl)-3-phenyl- (CA INDEX NAME)



RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

AN 1987:407151 CAPLUS

DN 107:7151

OREF 107:1319a,1322a

TI Heteroatom rearrangements. S,N, O,N, and N,N double rearrangements. X-ray molecular structure of 5-cyano-6-(methylthio)-2,3-diphenylpyrimidin-4(3H)-one

AU Yokoyama, Masataka; Hatanaka, Hidekatsu; Sasaki, Atsushi; Shiraishi, Tadashi; Kumata, Katsushi; Sakamoto, Kayoko; Ogata, Koreharu

CS Fac. Sci., Chiba Univ., Chiba, 260, Japan

SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1986), (7), 1187-96

CODEN: JCPRB4; ISSN: 0300-922X

DT Journal

LA English

OS CASREACT 107:7151

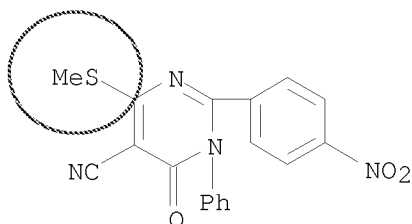
AB Cyclocondensation of MeSCR:C(CN)CONH₂ (I; R = OH) with R₁CO₂H (R₁ = Ph, 4-MeOC₆H₄, 4-ClC₆H₄, 4-O₂NC₆H₄, 2-naphthyl, 2-furyl) in the presence of P₂O₅-(Me₃Si)₂O complex gave oxazinones II in 49-79% yields. Reaction of I [R = NHPh] with R₁CO₂H (R₁ = Ph, 4-O₂NC₆H₄, 4-ClC₆H₄) under the same conditions gave pyrimidinones III and IV. The mol. structure of III (R₁=Ph) was determined by x-ray crystal structure anal. The reactions of I involve acylation of the cyano group, followed by transfer of the SMe group and ring closure.

IT 97242-70-1P 107427-92-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

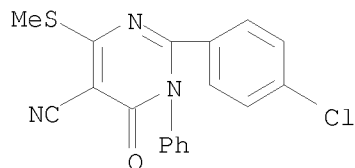
RN 97242-70-1 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1,6-dihydro-4-(methylthio)-2-(4-nitrophenyl)-6-oxo-1-phenyl- (CA INDEX NAME)



RN 107427-92-9 CAPLUS

CN 5-Pyrimidinecarbonitrile, 2-(4-chlorophenyl)-1,6-dihydro-4-(methylthio)-6-oxo-1-phenyl- (CA INDEX NAME)



L17 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

AN 1985:437445 CAPLUS

DN 103:37445

OREF 103:6075a,6078a

TI O,N and N,N double rearrangement

AU Yokoyama, Masatake; Hatanaka, Hidekatsu; Sakamoto, Kayoko

CS Dep. Chem., Chiba Univ., Chiba City, 260, Japan

SO Journal of the Chemical Society, Chemical Communications (1985), (5), 279-80

CODEN: JCCCAT; ISSN: 0022-4936

DT Journal

LA English

OS CASREACT 103:37445

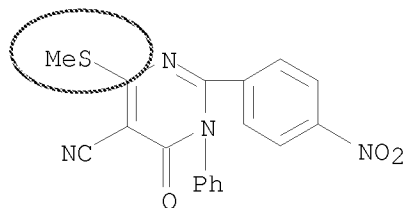
AB MeSCR:C(CN)CONH₂ (I; R = OH) condensed with BzOH in the presence of polyphosphoric acid trimethylsilyl ester (PPSE) gave 77% O,N-double rearranged product II (X = O), whereas similar condensation of I (R = NHPh) with BzOH in the presence of PPSE gave 49% N,N-double rearranged product III. Similar reactions occurred with other aromatic carboxylic acids and the mechanism of these heteroatom rearrangements are analogous to that of S,N-double rearrangement.

IT 97242-70-1P

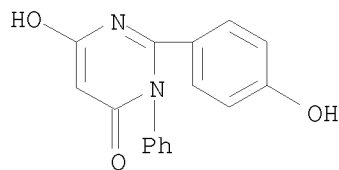
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 97242-70-1 CAPLUS

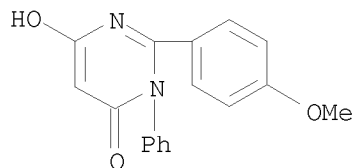
CN 5-Pyrimidinecarbonitrile, 1,6-dihydro-4-(methylthio)-2-(4-nitrophenyl)-6-oxo-1-phenyl- (CA INDEX NAME)



L17 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
 AN 1978:50401 CAPLUS
 DN 88:50401
 OREF 88:7945a,7948a
 TI Chemistry of imino esters and amidines. 11. Reaction of some amidines with malonating agents
 AU Shchavlinskii, A. N.; Samoletov, M. M.; Dashkevich, L. B.; Kul'bitskii, G. N.; Tarasov, B. P.
 CS Leningr. Khim.-Farm. Inst., Leningrad, USSR
 SO Izvestiya Vysshikh Uchebnykh Zavedenii, Khimiya i Khimicheskaya Tekhnologiya (1977), 20(9), 1319-22
 CODEN: IVUKAR; ISSN: 0579-2991
 DT Journal 102(b)
 LA Russian
 OS CASREACT 88:50401
 AB PhNHCR:NH (I; R = Ph) reacted with C3O2 at 35-40° or with malonic ester at 110-15° o give 70-85% (PhNHCR:NCO)2CH2 and 1-4% tetrahydropyrimidinedione II. Analogous treatment of I [R = 4-MeOC6H4, 3,4,5-(MeO)3C6H2] afforded the corresponding II in 60-83% yield. II exist as the enolized tautomers shown with intermol. CO...HO H bonds, according to their IR and NMR spectra.
 IT 65249-17-4P 65249-18-5P 65249-19-6P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and tautomerism of, spectra in relation to)
 RN 65249-17-4 CAPLUS
 CN 4(3H)-Pyrimidinone, 6-hydroxy-2-(4-hydroxyphenyl)-3-phenyl- (CA INDEX NAME)

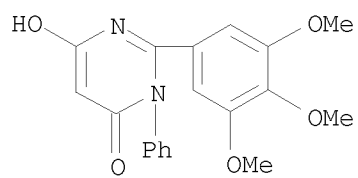


RN 65249-18-5 CAPLUS
 CN 4(3H)-Pyrimidinone, 6-hydroxy-2-(4-methoxyphenyl)-3-phenyl- (CA INDEX NAME)



RN 65249-19-6 CAPLUS
 CN 4(3H)-Pyrimidinone, 6-hydroxy-3-phenyl-2-(3,4,5-trimethoxyphenyl)- (CA INDEX NAME)

10/582,826



L17 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

AN 1957:39274 CAPLUS

DN 51:39274

OREF 51:7380a-i

TI Synthesis of 2,3,5,6-substituted 4-pyrimidones

AU Staskun, Benjamin; Stephen, Henry

CS Univ. Witwatersrand Johannesburg, S. Afr.

SO Journal of the Chemical Society (1956) 4708-10

CODEN: JCSOA9; ISSN: 0368-1769

DT Journal

LA Unavailable

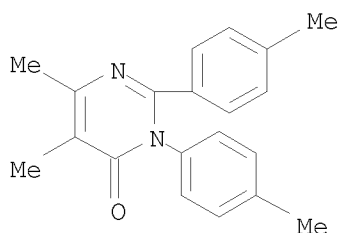
OS CASREACT 51:39274

AB 2,3,5,6-Substituted 4-pyrimidones (I) were readily synthesized by condensation of imidoyl chlorides (II) with Me or Et α -alkyl- β -aminocrotonates (III). The following general procedure was used: II (0.01 mole) and III (0.005, 0.01, or 0.02 mole) were refluxed 3-4 hrs. in 40 cc. dry CHCl_3 (method A) or allowed to remain at room temperature 2-3 days (method B). In some cases II and III were heated in the absence of a solvent (method C), HCl and alc. being evolved. The products were acidified with dilute HCl and steam distilled; this hydrolyzed any unchanged ester to steam volatile or H_2O soluble products, and converted unchanged II to the amide. After cooling, the latter was removed, and the filtrate treated with C and NH_3 deposited crude I which crystallized from dilute

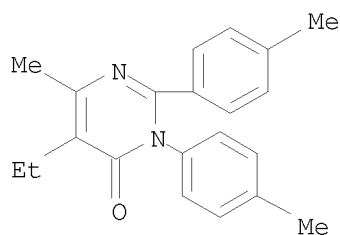
MeOH or alc. in colorless needles. The following I were prepared by the above methods (R and R substituents in II (RCCl:NR'), R' and X in III ($\text{MeC(NH}_2\text{):CR'CO}_2\text{X}$), molar ratio II:III, method, reaction temperature, reaction time in hrs., % yield, and m.p. given): Ph, Ph, Me, Me, 1:1, C, 140° , 0.5, -, -; Ph, Ph, Me, Et, 1:1, C, 140° , 0.5, 45, 157° ; Ph, Ph, Et, Et, 1:2, A, -, 4, 79, 159° ; Ph, o-C $_6$ H $_4$ Me, Me, Me, 1:1, A, -, 3, 53, 114° ; Ph, o-C $_6$ H $_4$ Me, Et, Et, 1:2, A, -, 4, 80, 152° ; Ph, m-C $_6$ H $_4$ Me, Me, Me, 1:1, C, 100° , 0.5, 31, 129° ; Ph, m-C $_6$ H $_4$ Me, Me, Et, 1:1, C, 100° , 0.5, 28, -; Ph, m-C $_6$ H $_4$ Me, Et, Me, 1:1, C, 100° , 0.5, 77, 136° ; Ph, m-C $_6$ H $_4$ Me, Et, Et, 1:2, A, -, 3, -, -; Ph, p-C $_6$ H $_4$ Me, Me, Me, 1:2, A, -, 3, 77, 146° ; Ph, p-C $_6$ H $_4$ Me, Et, Et, 1:2, B, -, 3, 75, 152° ; Ph, 2,4,1-Me $_2$ C $_6$ H $_3$, Me, Me, 2:1, A, -, 3, 83, 152° ; Ph, 2,4,1-Me $_2$ C $_6$ H $_3$, Me, Et, 2:1, A, -, 3, -, -; Ph, 2,4,1-Me $_2$ C $_6$ H $_3$, Et, Et, 2:1, A, -, 3, 83, 146° ; Ph, p-MeOC $_6$ H $_4$, Et, Et, 1:2, B, -, 3, 81, 161° ; Ph, p-MeOC $_6$ H $_4$, Pr, Me, 1:2, C, 155° , 0.5, 55, 163° ; Ph, m-O $_2$ NC $_6$ H $_4$, Me, Me, 1:2, C, 140° , 0.5, 62, 159° ; Ph, m-O $_2$ NC $_6$ H $_4$, Me, Et, 1:2, C, 140° , 0.5, 34, -; Ph, m-O $_2$ NC $_6$ H $_4$, Et, Me, 1:2, C, 140° , 0.5, 24, 160° ; Ph, m-O $_2$ NC $_6$ H $_4$, Et, Et, 1:2, C, 140° , 0.5, 38, -; Ph, 1-C $_{10}$ H $_7$, Me, Et, 1:2, A, -, 3, 64, 174° ; Ph, 2-C $_{10}$ H $_7$, Me, Et, 1:2, A, -, 3, 50, 189° ; Ph, 2-C $_{10}$ H $_7$, Et, Et, 1:2, A, -, 3, 40, 184° ; Ph, o-C $_6$ H $_4$ Cl, Me, Et, 2:1, A, -, 3, 13, 151° ; Ph, o-C $_6$ H $_4$ Cl, Et, Et, 2:1, C, 170° , 0.5, 32, 192° ; Ph, m-C $_6$ H $_4$ Cl, Me, Me, 1:1, C, 150° , 0.5, 35, 152° ; Ph, p-C $_6$ H $_4$ Cl, Et, Et, 1:2, C, 185° , 0.5, 59, 148° ; Ph, p-C $_6$ H $_4$ Cl, Pr, Me, 1:2, C, 185° , 0.5, 37, 154° ; Ph, Et, Et, Et, 1:2, B, -, 3, 73, 82° ; Ph, Et, Me, Et, 1:2, B, -, 3, 51, 118° ; o-C $_6$ H $_4$ Me, Ph, Me, Me, 2:1, A, -, 3, 80, 112° ; o-C $_6$ H $_4$ Me, Ph, Et, Et, 2:1, A, -, 3, 74, 137° ; p-C $_6$ H $_4$ Cl, Ph, Et, Et, 1:2, C, 155° , 0.5, 67, 146° ; p-C $_6$ H $_4$ Cl, Ph, Pr, Me, 1:2, C, 155° , 0.5, 21, 151° ; 3,4,5-(MeO) $_3$ C $_6$ H $_2$, Ph, Me, Me, 1:2, A, -, 3, 20, 181° ; 3,4,5-(MeO) $_3$ C $_6$ H $_2$, Ph, Et, Et, 1:2, A, -, 3, 37, 129° . The

synthesis of I was modified by preparing II by rearrangement of ketoximes (IV) with PC15. The following procedures were used. A solution of IV (0.01 mole) in 50 cc. CHCl₃ was treated at 0° with 0.01 mole PC15, the whole shaken 1-2 min., and the solution treated by one of the following procedures. The solution refluxed 15 min. to complete the rearrangement of IV, the III (0.02-0.03 mole) added in 10 cc. CHCl₃, and reflux continued 2-3 hrs. (method D). Alternatively, the solution after remaining 2 hrs. at room temperature was cooled to 10°, the III (0.02-0.03 mole) in 10 cc. CHCl₃ added, and the mixture left 1-2 days at room temperature (method E). The following method (F) gave good yields of I. The solution of rearranged IV, after 2 hrs. at room temperature was distilled at 40-5°/30 min., then stored 1-2 days with 0.02-0.03 mole III, and the products treated as previously described. I were crystallized as colorless needles from MeOH or alc. The following results were obtained (IV, R' in III, method, % yield, and m.p. of I given): PhMeC:NOH, Et, E, 65, 126°; (p-MeC₆H₄)MeC:NOH, Et, E, 65, 82°; (p-MeC₆H₄)MeC:NOH, Me, D, 65, 146°; 2-C10H₇CMe:NOH, Et, F, 65, 130°; PhPrC:NOH, Et, E, 72, 106°; PhPrC:NOH, Me, E, 35, 73°; (p-MeC₆H₄)₂C:NOH, Me, F, 73, 128°; (p-MeC₆H₄)₂C:NOH, Et, F, 60, 140°; Ph₂C:NOH, Et, D, 55, 157°. Improved yields of I were obtained by using excess II or III.

IT 102316-51-8P, 4(3H)-Pyrimidinone, 5,6-dimethyl-2,3-di-p-tolyl-
 102660-46-8P, 4(3H)-Pyrimidinone, 5-ethyl-6-methyl-2,3-di-p-tolyl-
 102660-83-3P, 4(3H)-Pyrimidinone,
 5,6-dimethyl-3-phenyl-2-(3,4,5-trimethoxyphenyl)- 102810-25-3P,
 4(3H)-Pyrimidinone, 5-ethyl-6-methyl-3-phenyl-2-(3,4,5-trimethoxyphenyl)-
 103755-10-8P, 4(3H)-Pyrimidinone,
 2-(p-chlorophenyl)-6-methyl-3-phenyl-5-propyl- 109809-97-4P,
 4(3H)-Pyrimidinone, 2-(p-chlorophenyl)-5-ethyl-6-methyl-3-phenyl-
 110144-94-0P, 4(3H)-Pyrimidinone, 5,6-dimethyl-3-phenyl-2-o-tolyl-
 110244-34-3P, 4(3H)-Pyrimidinone,
 5-ethyl-6-methyl-3-phenyl-2-o-tolyl-
 RL: PREP (Preparation)
 (preparation of)
 RN 102316-51-8 CAPLUS
 CN 4(3H)-Pyrimidinone, 5,6-dimethyl-2,3-bis(4-methylphenyl)- (CA INDEX NAME)

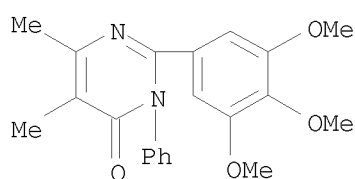


RN 102660-46-8 CAPLUS
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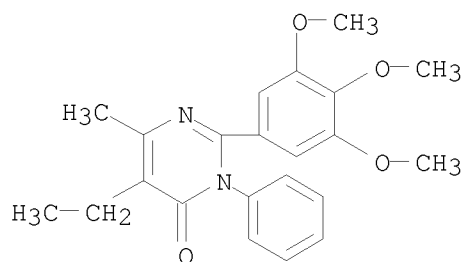
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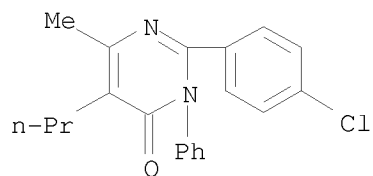
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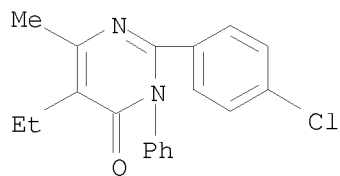
RN 103755-10-8 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(4-chlorophenyl)-6-methyl-3-phenyl-5-propyl- (CA INDEX NAME)



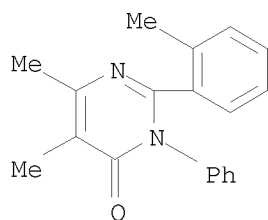
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CN 4(3H)-Pyrimidinone, 2-(4-chlorophenyl)-5-ethyl-6-methyl-3-phenyl- (CA INDEX NAME)



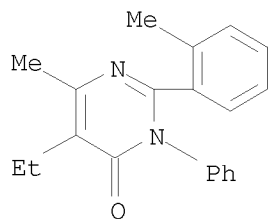
RN 110144-94-0 CAPLUS

CN 4(3H)-Pyrimidinone, 5,6-dimethyl-2-(2-methylphenyl)-3-phenyl- (CA INDEX NAME)



RN 110244-34-3 CAPLUS

CN 4(3H)-Pyrimidinone, 5-ethyl-6-methyl-2-(2-methylphenyl)-3-phenyl- (CA INDEX NAME)



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COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

96.88

288.74

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-13.94

-13.94

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